Hrvoj Vančik

From Complexity to Systems

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Dedicated to my parents

Preface

My interest in the problem of complexity appeared during the period when my scientific activity focused on the development of a new field of physical organic chemistry and the study of the reaction mechanisms in crystals and in the polycrystalline phases. In contrast to the reactions in solution, for which the kinetic behaviour in most cases affords the exponential growth of the product, reactions in crystals behave in much more complicated ways. Before all, these processes are the combination of two transformations. First one is the chemical reaction which is manifested as the change in chemical bonding, and the second process is the phase transformation of intermolecular arrangements. From these investigations, I have learned that such processes are not simple. Rather, they are interrelated systems of transformations. I have found that this idea is a general principle by which most of the natural processes behave as systems, and that these systems are complex. From the experimental point, the phase transformation kinetics are described with the sigmoidal curve which represents the correlation of the growth of the product phase *versus* the time of the reaction. Analogous kinetics described with the sigmoid growth were observed also for a series of complicated reactions such as the autocatalytic processes. In such autocatalytic processes, the product of the reaction enhances the rate of its own formation. This feedback appears to be one of the basic principles of the functioning of systems. I have found that these studies in chemistry, if they are observed from a wider angle, belong to the more general scientific problems: the problem of complexity and the problem of systems.

By consulting the literature, the readers could be confused because the concept of complexity and the concept of systems are in some cases represented as the same basic idea, and in other examples as two phenomena. Some of the books in this field, such as the book by Klaus Mainzer "Thinking in complexity", were oriented to the complexity used as a *terminus technicus*, but on the other side, we have the book by Karl Ludwig von Bertalanffy entitled "General system theory" in which the focus is to the systems. Both of the works talk about both of the notions, the system, and the complexity without an explanation of whether the system theory and the theory of complexity are the same or not, or, at the least, to which extent they overlap.

The first concept about the relationship between complexity and systems has appeared as an *Ars brevis* in my paper with the same title, published recently in Foundations of Chemistry [1]. In this book, I wish to propose the framework within which the phenomenon of complexity could be explained through the construction of a specific classification. By using this classification, the previously confused explanation of the complexity, or the various kinds of complexities, becomes more systematic. In this classification, the complexity of any entity can be represented within a sort of the "complexity space", the combination of the three different contributions: synchronic, diachronic, and combinatorial complexity. Starting from this approach, the research is extended with the discussion about the possibility of limits in complexity. Accordingly, the central question is whether complexity can grow *ad infinitum*, or whether there is a sort of limit, or a sort of "attractor point" to which complexity could converge. The possibility of the constraints in the complexity of the natural structures such as molecules or living beings is studied starting from the idea that the synchronic complexity has a sort of the level structure. This level structure is ordered hierarchically from subatomic particles to atoms, molecules, supramolecules, etc. I argue that when we go to the higher level structures, their stability diminishes, and the complexity approach to the limiting chaos.

The main problem in the discussion about combinatorial complexity is the relationship between complexity and diversity. Because for the measure of diversity I use the Shannon entropy, the relationship between complexity and diversity is reduced to the relationship between complexity and entropy. Growth of the combinatorial complexity is frequently modelled by using the fractal representation. Starting from this fact, I developed the theoretical approach to complexity by studying its possible constraints by analysing the combination of fractal representation of complexity in which the fractal dimension, Shannon entropy, Golden Ratio, and the first Feigenbaum constant are correlated. The basic conclusion is that the maximum complexity does not correlate with the maximum diversity.

Complexity of natural entities analysed in such a way serves as a starting point for the investigation of systems. In this discussion, complexity and systems are defined in the following way: while complexity is regarded as a property, the state of organization, the system is an object. System is formed from the spatiotemporal entities, the natural items for which I use the name actual entity or actuality. This term is borrowed from the metaphysics developed by Alfred N. Whitehead in which events rather than objects form the actual Universe.[1] These actualities that are characterized by corresponding combination of their synchronic, diachronic, and combinatorial complexities can be interconnected to each other to form the system. As it will be discussed at the end of this book, actualities can be also the systems. Formation of the system is the consequence of the impact of the environment, and this impact appears as the requirement to perform a particular function. Thus, the formation of systems

[1] The alternative term for the components of systems, the *enion*, has been proposed by Strevens in his analysis of the nondecomposable systems, Ref [1].

is directed teleologically. For the representation of systems in this book I used the method that has been developed within the field of the chemical graph theory. I show that the graph-theoretical approach could be helpful for the explanation of the basic principles of the theory of systems, especially homeostasis, and equifinality.

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Reference

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Chapter 1
Introduction

In the middle of the last century, Alan Turing, who is known as one of the founders of computers and the information theory, as well as one of the pioneers of the science about the artificial intelligence, has published the work in which he demonstrates how the simple combination of just a few chemical reactions together with the diffusion processes can spontaneously result with the appearance of the morphological patterns similar to the simple biological forms [1]. In this paper Turing has initiated the discussion about two concepts in the same time: the concept of complexity, and the concept of systems. Although both the disciplines, the science of complexity, and the science of systems, have appeared within the same historical period during the first half of the last century, their interrelations were not satisfactory studied and analysed. By superficial view, both of the approaches are based on the same principles of the holistic behaviour of the ensembles consisting of particular components. In the largest part of the available literature, the *theory of complexity* can be recognized in the form of *the theory of chaos* [2]. *Inter alia*, this theory has in the history of science emerged almost simultaneously from the investigations in different fields. For the example, one of such fields is the mathematical modelling of atmospheric dynamics developed by Edward Norton Lorenz. Independently, the oscillating as well as the chaotic behaviour, both were discovered also in other fields of science, chemistry, biology, social sciences, etc. An excellent example can be found in chemistry with the outstanding work of Belousov and Zhabotinsky on the discovery of chemical oscillators. They have found that the collection of coupled chemical reactions can under particular circumstances behave either regularly or chaotically, depending on the conditions of medium and strongly depending on the starting conditions.

In biology, as well as in demography, the development of populations is described by using the nonlinear dynamical equations. This representation is known as a *logistic map*. The idea has appeared when Robert May [3] has described the growth of population by using the equation:

$$x_{n+1} = \lambda x_n(1 - x_n)$$

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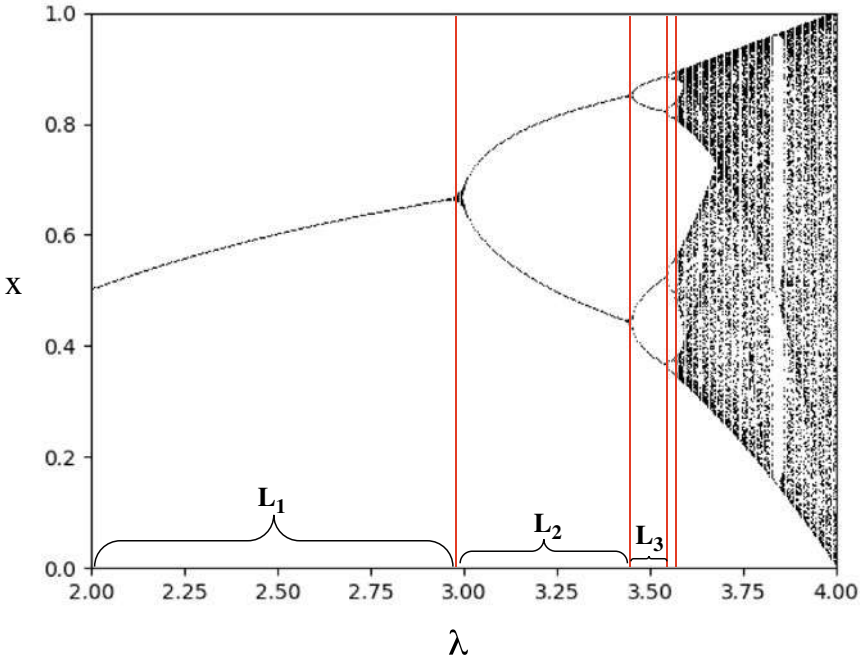

Fig. 1.1 Logistic map for the growth of population **x** in the dependence of the parameter λ. Perpendicular red lines represent the characteristic values when the bifurcation of **x** led either to complex oscillations or to chaos. (adjusted from the public web page https://www.sci-pi.org.uk/maths/logistic.html)

In this equation the variable x_n represents the extent of the growth of population, and it appear within the interval from 0 to 1. The graphic representation or this equation is shown in the Fig. 1.1. The fate of the population depends on the value of the parameter λ. The characteristic values of λ are in Fig. 1.1 labelled with the perpendicular red lines. If λ lies between 0 and 1, the population will die. Higher λ led either to the linear growth (λ is between 2 and 3), or to the regular oscillations between two values (λ is between 3 and 3.449), or between four, eight, et. values (λ is between 3.449 and 3.544). These values of λ are known as the *bifurcation points.* If λ is larger than 3.5699 the oscillations become chaotic. Mitchel Feigenbaum has found that the ratio L_n/L_{n+1} (for example L_1/L_2, or L_2/L_3 in the Fig. 1.1) is constant independently on the starting conditions. This ratio in known as the first Feigenbaum constant which is equal $\delta = 4.66920\ldots$The second Feigenbaum constant, α, defines the ratio between the widths of the neighbouring bifurcations on the red lines ($\alpha = 2.50290\ldots$) (Fig. 1.1).

This approach has been one of the basic concepts for the appearance of the theory of chaos in the form as it was formulated by Mitchell Feigenbaum and Benoit Mandelbrot.

The idea about complexity can be extended from studies of the dynamical systems to other aspects of scientific investigations. We could also talk about the complexity of structures, complexity of the hierarchical construction of the universe, complexity of computer programs, etc. Thus, the new field of transdisciplinary science has been conceptualized! However, the thinking in complexity is not oriented exclusively to science. Rather, how I will demonstrate on the end of this book, it can explain the deep connections between science and art [4].

Almost in the same time, during the middle of the last century, the biologist Karl Ludwig von Bertalanffy has proposed another trans-discipline, the *theory of systems*. Using biological systems such as the growth of organism as well as the stream of the evolution of life as the starting models, Bertalanffy has proposed the general theory that could be extended to the description of a wide variety of natural or artificial systems. It appears not only in natural science, but also in psychology, or even in economy and managerial applications [5]. Since the theory of complexity has also been mostly discussed within the frame of the dynamical behaviour of systems, its resemblance to the general system theory invented by K. L. von Bertalanffy is obvious [6]. The research about the science of complexity and the science of systems has been accelerated after the establishment of the Santa Fe Institute in 1984, on the initiative of the physicists David Pines and Murray Gell-Mann. The focus of the research program of the Institute includes, *inter alia*, the investigations of so called *complex adaptive systems* (CAS). However, from the vast literature that has been emerged from the Institute it could be recognized that the differentiation between the notion of complexity and the notion of system has not been defined unequivocally [7]. The confusion about the problem of complexity and the theory of systems can be recognized in the discussions about the levels of complexity in philosophy of science. For instance the concept of the level structure of the complexity, which will be discussed in details later in this book, has been criticised with the argument that the objects on the higher level of complexity are not exclusively composed of the objects on the immediate lower level [8]. For instance, ecosystems are not composed only of the organisms but also of the waste, inorganic compounds, physical transformations, etc. The problem in this criticism is in the mixing of the notion of complexity and the notion of systems. Ecological *systems* are composed (and influenced) from the components of various levels of complexity. It is not the *complexity* that is composed of various complexities. In this work I propose the representation based on the graph theory in which the systems are composed from components (which can also be smaller systems) of different complexity.

In this book, I am trying to generalize the theory of complexity by elaborating all the observable manifestations of complex forms and behaviours, and, in addition, to explain how it is related to the general theory of systems. In principle, I argue that the system represents a higher degree of complexity, say, a sort of meta-complexity whose nature emerges as a combination of the contributions of different complex entities. Or, by simpler words, while complexity could be imagined as a sort of property, systems are the teleological objects, that are formed to accomplish particular functions.

In the book "The End of Science", its author John Horgan refers to his correspondence with professor Seth Lloyd about the problem of complexity. In the appendix of the Horgan's book, we can read about the response of professor Lloyd in which no more no less but 45 definitions of complexity were proposed [9]. Consequently, the phenomenon of complexity should necessary be redefined on the more systematic way. First of all, from the aspect of the rigorous science, complexity should be deliberated by using different scientific methodologies.

In this book I propose that the concept of complexity should be systematized through the consideration of three categories: synchronic, diachronic, and combinatorial complexity. Thus, the complexity of every natural or artificial entity is expressed as a combination of the contributions of three components: synchronic, diachronic, and combinatorial. In chemistry, we can find the typical examples for all of these contributions. Since the basic concept about complexity is naturally related to the concept of diversity, the unavoidable questions that emerge are about the relationship between complexity and entropy (understood as a measure on the order-disorder scale) [10, 11]. The interplay between disorder, diversity, entropy and complexity is in this book discussed from various aspects. First of all, I examine these relationships within the frame of the theory of cellular automata by Stephen Wolfram [12] and within some aspects of the general information theory developed by Claude Shannon. Within these aspects, it is proposed that maximum of complexity could be considered not as the state of the maximal diversity, but rather as a degree of organization. Complexity regarded as a degree of order can reach its maximum which is between the homogeneity and chaos. This maximum of complexity is the state whose minimal variation causes maximal change in the information entropy.

The special questions that appear in the studies about complexity are focused on the quantification of complexity and on the possibility of its limited or unlimited growth. Here, the central question is whether absolute simplicity or absolute complexity exist at all? Chemistry as a central science can provide a series of the examples that can serve as convenient models in this examination.

The first step in the explanation of the relationship between two theories, the theory of complexity, and the theory of systems, is the construction of convenient representations. The main criterium in constructing of such representation should be to achieve its appropriate explanatory power. In this book I propose the representation of the complexity of objects (I use also the term "entities") by using the "quasi-coordination diagram" in which the "coordinates" are associated to different types of complexity. The term "quasi-coordination diagram" means that the coordinates of complexity are not labelled with any sort of distinct metrics, i.e., they are without units. The entities (objects) are inherently complex and their complexity is described as a combination of the different contributions of three components: synchronic, diachronic, and combinatorial. The formation of systems involves the specific interconnections between these complex entities. Particular combination of the connections between the objects, by which the system is created, is the consequence of the impacts of the environment. In the systems formed in such a way, the components (entities, objects, actualities) interconnect each other on a specific way to satisfy particular environmental requirements, which are manifested as the

requirement for performing of certain function. Theoretically, this network of the specifically interconnected entities can be conceived as a sort of the topological structure. The topological objects are routinely studied by using the representations developed in the graph theory. It is very well known that the graph theory is frequently used for the representation of chemical structures of molecules, especially for their constitutions. As such, chemical graph-theoretical methods are widely applied in exploring the structure–property correlations.

The use of the basic graph theory for the representation of the structure of systems, which are formed by various interconnections of complex entities, the actualities, can provide the deeper insight into the philosophical problem about the nature of the influence of the environment, independently whether we talk about the environment as natural function, or if we talk about the more "technical" type of the environment which requires the formation of corresponding function that is in the core of the design of new technological components. From the represented discussion, it becomes possible to propose the clear-cut difference between two categories, category of complexity and category of systems. While complexity should be considered as a sort of property (or the state of organization), systems are in principle teleological objects fashioned to accomplish particular function. However, the theory of complexity and the theory of systems are overlapped, they are in principle the same theory.

References

1. Turing AM (1952) The chemical basis of morphogenesis. Philos Trans R Soc Lond Ser B Biol Sci 237(641):37–72
2. Mainzer K (1994) Thinking in complexity. Springer-Verlag, Berlin, Heilderberg
3. May RM (1972) Will a large complex systems be stable? Nature 238(5364):413–414
4. Taylor R (2003) Fractal expressionism—where art meets science. In: J Casti, A Karlqvist (eds) Art and complexity. Elsevier Science B.V
5. Mele C, Pels J, Polese F (2010) A brief review of systems theories and their managerial applications. Serv Sci 2:126–135
6. von Bertalanffy KL (1969) General system theory. G. Braziller, New York
7. Gell-Mann M (2003) Regularities and randomness: evolving schemata in science and the arts. In: J Casti, A Karlqvist (eds) Art and complexity. Elseiver Science B.V
8. Guttman B (1976) Is 'levels of organization' a useful biological concept? Bioscience 26(2):112–113
9. Horgan J (1997) The end of science (Note 11). Broadway Books, New York, p 203
10. Shannon C, Waever W (1949) The mathematical theory of communication. University of Illinois Press, Urbana
11. Li W (1991) On the relationship between complexity and entropy for Markov chains and regular languages. Complex Systems 5:381–399
12. Wolfram S (2002) The new kind of science. Stephen Wolfram, LLC

Chapter 2
Concept of Complexity

Since in the scientific history, the term *complexity* has to some extent been associated to the term *chaos*, in the vast literature about these phenomena the basic principles of the theory of complexity can be found in the works about the theory of chaos. In his book "The End of Science", Horgan has proposed the use of the term "chaoplexity" [1]. The earliest period in the historical development of the theory of complexity has emerged during the discoveries of time-periodic processes that can behave either regularly or quasi-regularly, of chaotically. The pattern of this behaviour is strongly dependent on the impacts of environment. In the mathematical description of these processes, the influence of the environment is represented through the variations of different controlling factors which appear in the differential equations. These controlling factors can be physical quantities such as temperature, the rate of flow, etc. However, many of these controlling factors (such as Feigenbaum constants), [2] are not in the relation with any of the particular physical or chemical parameters. Rather, they are universal.

The study of the complexity in chemistry has emerged from the discovery of the oscillating reactions of which the mostly investigated are the Belousov-Zhabotinskii oscillations [3]. On the other hand, the term *complexity of molecules* came into the view as a result of the investigations of the relationship between the molecular structure as it is represented by chemical formulas, and the physical or chemical properties of corresponding substances. One of the most exploited methods that have been applied in these investigations is chemical graph theory. This approach has an important role especially in the search for the substances which could be important for pharmaceutical industry. Thanks to the availability of the fast computers, it is possible to find the small group of molecular structures which afford specific properties required for their medical activity simply by analysing the data bases which consist of the large number of possible structures represented by constitutional molecular formulas. This approach is very well known as the QSAR approach (**Q**uantitative **S**tructure–**A**ctivity **R**elationship) [4].

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Let me focus now to the wider view, the more general questions about complexity. One of these important questions is about the complexity of sciences, or, more precisely, the complexity of scientific disciplines. For the instance, why it is generally accepted that biology is more complex than physics of elementary particles? In particular, why are the subjects investigated within biology more complex than the subjects studied within physics? Generally, how to classify the complexity of the phenomena which are in the focus of different scientific fields. This question is of the basic importance in the philosophy of science because it is in the heart of the problem about the autonomy of specific scientific disciplines. From the radical reductionistic statement, all the sciences can be reduced to physics, and all the laws of the special sciences are derivable from the laws of physics [5]. In contrast, holistic view is based on the opinion that sciences, such as biology, chemistry, etc., are to some extent autonomous and that they have formulated their own laws and concepts that are not immediately derivable from the laws of the physics of elemental particles.

From one of the reductionistic views, sciences are divided in two groups: intensive sciences and extensive sciences [6, 7]. While intensive sciences are in the search for the fundamental laws of the nature, the activity of extensive sciences is focused on the exploration of the actual and specific natural phenomena. Thus, these laws formulated within the intensive sciences serve for the formulation of the heuristic base of the extensive sciences. As we will discuss in the following chapters, both the concepts are true, taking into account that every scientific discipline comprises two sides, the scientific ontology and the scientific epistemology. From the ontological point of view, the properties and behaviour of all the known substance strongly depend on the properties and characters of fundamental particles and interactions. The Universe would look quite differently if, for instance, the charge of electron would be modified. On the other hand, the epistemology could be regarded as the scientific method which helps to get the deep insight into the essence of the matter. Scientific disciplines which have been developed through the history of science differ in their epistemologies. For instance, it is difficult to derive the laws of organic reaction mechanisms from basic equations of quantum mechanics because the theory about reaction mechanisms exclusively belongs to chemical epistemology. There are no organic reaction mechanisms on the level of the elemental particles. Similarly, how to derive social behaviour of animals from the chemical and/or biochemical concepts that explain their basic biological activity? However, it must be pointed out that even from the epistemological point, the physical theories are to some extend privileged in the relation to the theories of the higher level sciences. In this sense, the "higher-level theories" such as chemical or biological concepts cannot be in conflict with the basic physical principles [8].

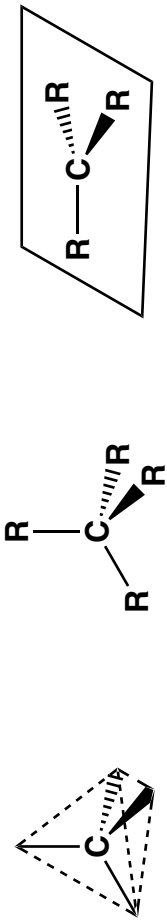
Starting with the idea that the main intention of science is the development of methods for the interpretation of natural appearances, epistemological approach which forms these interpretations should be the origin of the division of science to special disciplines. Thus, the hierarchy of sciences is fundamentally epistemological, it is the result of the historical development of the knowledge. In this hierarchy,

physics appears on the most fundamental level, followed by chemistry, biochemistry, biology, etc. The reason why such special scientific disciplines have developed their peculiar epistemology lies in the *complexity of their objects of investigation.* Molecules are more complex than atoms, living beings are more complex than molecules, etc. This fact implies that this hierarchy is the mirror picture of the complexity of matter, which has a level structure. The problem that will *inter alia* be discussed in this book is about the representations of complexity and complex systems. In the rigorous science the unavoidable tool for the representation of the empirical facts is the mathematical approach, especially the use of the statistical approach. It is important to point out that the mathematical representation is universal, not dependent on the hierarchy of complexity [9].

The discovery of complex reaction systems such as Belousov-Zhabotinski oscillator is not the only example of the role of chemistry in the historical development of the theory of complexity and the theory of chaos. One of the basic concepts in the chemical epistemology is *structural theory* which reveals the *constitution* of molecules from atoms, i.e., how the atoms are interconnected between each other to form the molecule. Thus, this structural theory is conceptually topological. More sophisticated view on the molecular structure is the 3D spatial distribution of atoms from which we get the information about the real shape of the molecule, the molecular *configuration*. From the more rigorous point of view within quantum mechanics, atoms in molecules are constantly in vibrational movements, and, consequently, there is no molecular shape. Molecular three-dimensional structure is the concept that belong to the chemical epistemology, and it emerges only after the use of the Born–Oppenheimer approximation.

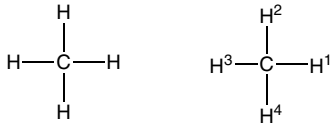
The 3D structure, or the configuration of molecules has been discovered independently by vant'Hoff and LeBell. In one of the classes of organic molecules, the saturated hydrocarbons, the molecules consist of the interconnected carbon atoms. These atoms are bound to other atoms or between each other in such a way that the lines of chemical bonds outgoing from each carbon atom are oriented to the vertices of tetrahedron (Fig. 2.1a, b). In the class of the unsaturated hydrocarbons, the shape of the molecule is different. They are characterized with the another type of the structures in which the carbon atoms are not in the centre of the tetrahedron. Rather, they are coplanar with the neighbouring atoms (Fig. 2.1c). Thus, the carbon atom appears either in the centre of the tetrahedron, or in the same plane with other neighbouring atoms.

Since the atoms in molecules can be interconnected on the innumerable ways, the molecular structures can be spread through a vide scale of complexity. As we have just represented, the structures of molecules, their constitutions are on the simplest way represented by *constitutional formulas* in which the symbols of atoms are connected by lines. For instance, the molecule of methane (Fig. 2.2) is represented by formula which provides its unequivocal *description.* Since the constitution of the real molecule of methane is simple, its description by formula CH_4, with the meaning that "C is bound to H^1, H^2, H^3, and H^4, and there is no bond between these H atoms", is also simple. More complicated is the structure of another molecule (benzene), and it will take some time to figure out the verbal description of its constitution formulated



A B C

Fig. 2.1 Typical configurations of organic molecules: **A**, and **B**, tetrahedral, **C**, coplanar. **R** stands for any kind of atom

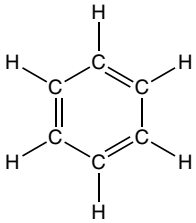


Constitution of the methane molecule

DESCRIPTION

C is bound to H^1, H^2, H^3, H^4

There is no bound between H^1, H^2, H^3, H^4



Constitution of the benzene molecule

DESCRIPTION
?

Fig. 2.2 Constitutions of molecules represented by chemical formulas, and their descriptions

as C_6H_6. Thus, it is not only the structure of the benzene molecule more complex than the structure of the methane molecule, but also the *description* of benzene molecule is more complex than the *description* of the methane molecule! From this example we have discovered that the possible measure of *complexity of entities* (in our case molecules) is the *complexity of their descriptions*. This fact will be discussed in more details in the chapters that follow.

Since the molecules are spatial objects, their shape is also characterized with corresponding properties of *symmetry*. The simplest definition of symmetry is the invariance of the object regarding to specific spatial operation (reorientation). For instance, if we rotate the cube around its vertical axis for 90 degrees, it will look the same. Say, the cube possesses the symmetrical element called the axis of symmetry. In addition, if we intersect the cube with a plane, the left and right side will mirror each other. The symmetrical plane and the symmetrical axis belong to the *elements of symmetry* which are shown in Fig. 2.3.

We could say that an object is more symmetrical if it possesses more symmetry elements. For example, the cube in Fig. 2.3 is highly symmetrical solid with, *inter alia*, three planes and three axes of symmetry. In geometry, the most symmetrical solid is the sphere. Deformation of the solid, for instance by transforming the cube to cuboid shape, results with the loss of particular symmetry elements.

Such diminishing of the symmetry, the *break in symmetry*, is one of the key characteristics of the change in complexity. As the object is less symmetrical, it becomes more complex. However, this rule requires deeper insight into the problem of complexity by analysing more sophisticated structures and dynamics.

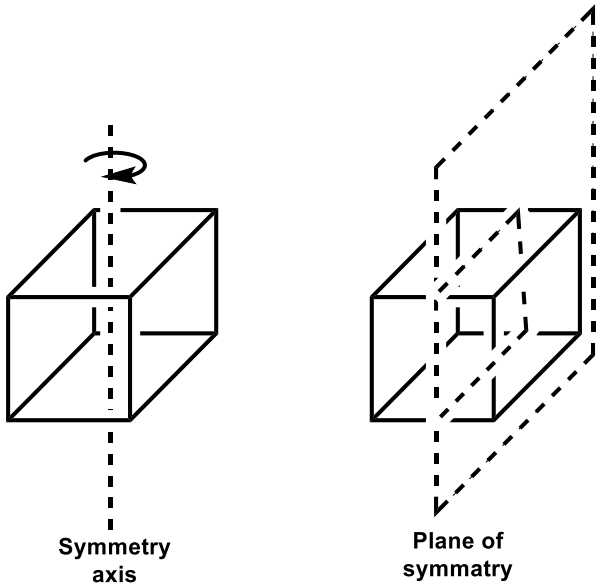


Fig. 2.3 Some elements of symmetry of the cube

Break in symmetry of molecules is very well known in chemistry as the appearance of the molecular *chirality*, or *handedness* of the shape of the molecules of products of some chemical reactions. The simplest explanation of chirality is following. If the molecule and its mirror image cannot be overlapped then this molecule is chiral. Analogously, while the left hand is the mirror image of the right hand, it is not possible to overlap the hands by any reorientations in the space. In molecules, while molecule **A** in Fig. 2.4 can easily be overlapped with its mirror image, molecule **B** cannot be overlapped with its mirror image in any way. Thus, transforming the structure **A** to the structure **B** results in the loss of symmetry, the symmetry break. Since the molecule **B** is chiral it is more complex than the molecule **A**. Similarly, in going from the structure **C** to the structure **D**, the complexity increases because **D** is chiral, and it does not possess the plane of symmetry labelled as the dotted line in Fig. 2.4.

Appearance of handedness (chirality) in chemical evolution has been the essential step for the emergence of life. Of the two possible configurations of the chiral amino acids, labelled as L, and D, respectively, the amino acids which are isolated from living organisms have predominantly the L configuration. Thus, it is important to point out that the beginning of life is the immediate consequence of the break in symmetry in which the D amino acids are eliminated from the "primordial soup of life" (Fig. 2.5).

Now, the question is how such a symmetry break can appear in chemical evolution? Is it possible that this process occurs spontaneously? Could it be expected that the formation of the chiral molecular structures is a consequence of corresponding types of chemical reactions? In the example represented in Fig. 2.6, the chiral structure

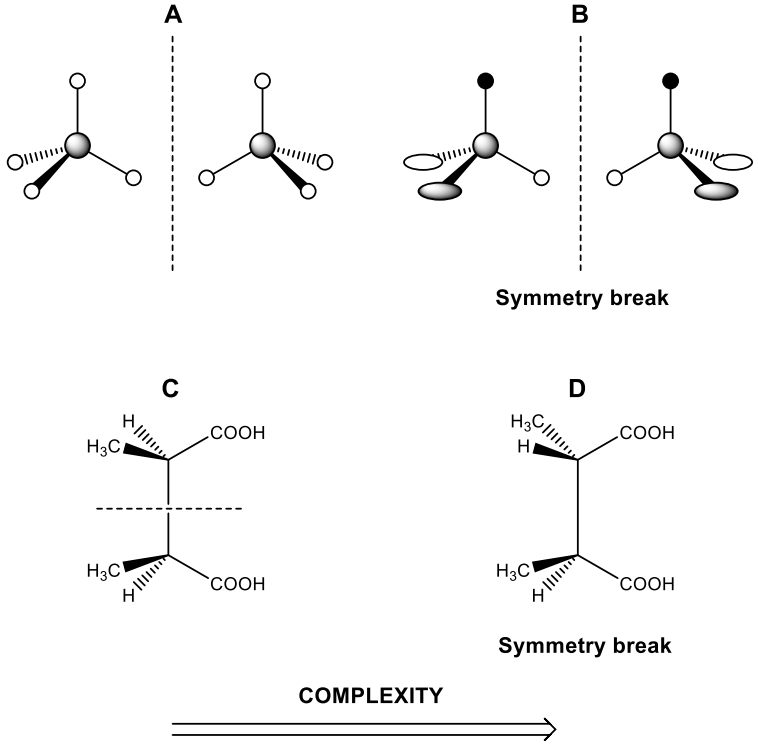


Fig. 2.4 Break in symmetry in molecules. The structures **B** and **D** are less symmetrical, i.e., they are chiral, because they cannot be overlapped with their mirror images (labelled with the perpendicular dotted lines) and, correspondingly, they are more complex

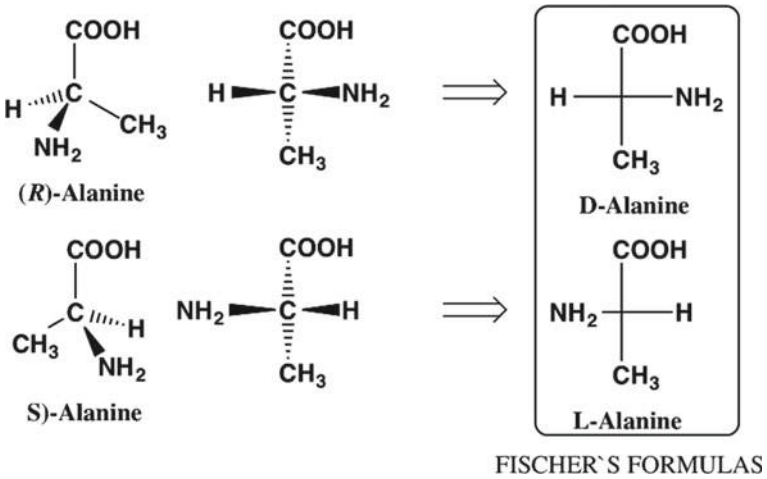


Fig. 2.5 Break in symmetry in amino acids. In all the living systems dominate the L amino acids

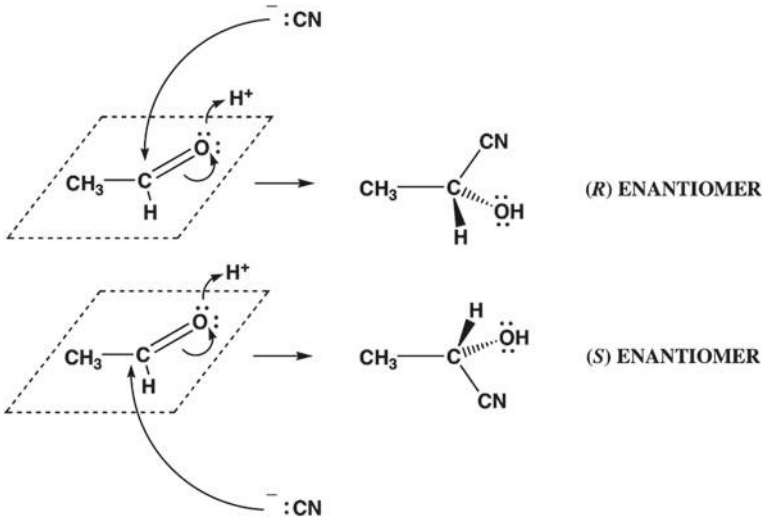


Fig. 2.6 Mechanism of the addition of the CN- ion to the carbonyl group (C = O) of the aldehyde. Since aldehyde molecule (on the left side) is planar, it is not chiral. After the CN- addition, the molecules on the right side (the products) appear as two chiral forms, the (*R*) and (*S*) enantiomers

of the *product* of the reaction is the result of the chemical reaction in which the molecule of cyanide ($CN:^-$ in the Figure) adds to the molecule of aldehyde.

The starting substance, the *reactant* in this chemical reaction is acetaldehyde. By the detailed inspection in its molecular structure (left structures in Fig. 2.6) we can observe that atoms C (from the CH_3 group), O, and H lie in the same plane with the central atom C. Since this plane is at the same time the plane of symmetry, this molecule is not chiral. The detailed inspection to this structure would show that it overlaps with its mirror image. All the spatial structures of the objects which have at the least one of the planes of symmetry are not chiral! In the represented reaction, another reactant, the cyanide, $CN:^-$, can form chemical bond with the central C-atom of acetaldehyde. In this reaction the $CN:^-$ molecule can approach to the plane in which lie the atoms of the acetaldehyde molecule from two sides. Depending whether $CN:^-$ approach from above, or from below this plane, the products (on the right side of Fig. 2.6) have the opposite chirality labelled with (*R*) and (*S*). Namely, because the structures of the product molecules of this reaction are three-dimensional (they have the tetrahedral form with the C-atom in the centre of the tetrahedron) without the symmetry plane, they are interrelated as the object and its mirror image, i.e., they are chiral. This reaction is the example of the chemical break in symmetry that forms the left-hand and the right-hand shaped molecules, so called (*R*) and (*S*) isomers, which are in chemical terminology known as the *enantiomers*. In the laboratory or in the nature, this reaction can proceed in some closed vessel in which the large number of molecules exists. Consequently, the resulting substance in this reaction vessel is the mixture of both enantiomers ((*S*) and (*R*)) in the *equal*

amounts. Such mixture is called the *racemate*. The equal amounts of the (*R*) and (*S*) isomeric products appear because the probability of the CN:$^-$ molecule to approach to aldehyde molecule from above, or from below of the molecular plane of aldehyde is equal. Consequently, in such *macroscopic* real chemical systems, the reaction always finishes with the formation of the racemate, and there is no macroscopic break in symmetry in this reaction vessel. However, the appearance of life is possible only in the reaction systems in which only one of the enantiomeric products is predominant. How it is possible if all the reactions led to the racemate on the way how I have explained immediately?

Since one of the basic characteristics of the living systems is that they can produce only one of the enantiomeric forms of the molecules involved in biochemical processes, the transition from non-living to living systems requires some additional environmental impacts which can induce the break in symmetry, i.e. which can destroy the racemate.

The explanation we can find by examining the mechanisms of the chemical reactions occurring in living organisms, the mechanisms of biochemical reactions. Let us use, for example, the biochemical reaction of the biosynthesis of L-glutamic acid (Fig. 2.7). Characteristics of biochemical processes in living organisms is their complexity because these reactions in most of the cases occur only with the help of catalyst. The catalyst which promotes the reaction shown in Fig. 2.7, is the enzyme *aminotransferase*. One of the most important properties of the enzyme catalysts is that they have the characteristic spatial structure with the *chiral cavity* in its active centre, and only one of the enantiomers can form the complex with such catalyst molecule. In the biochemical textbooks the bonding of the reacting molecule with the active centre of the enzyme molecule is figuratively explained with the key-lock analogy. Thus, the catalytic function of aminotransferase is, *inter alia*, the *transmission of the chirality* of the active centre of the enzyme catalyst to the chirality of the product molecule in this reaction. Consequently, only the L-form of the glutamic acid is produced (Fig. 2.7).

From this example we learn that macroscopic chirality (i.e., the excess of only one enantiomer) cannot be obtained spontaneously but only by the *impact from outside*, in this case by the influence of the chiral enzyme catalyst. If the symmetry break is the essential step for the increase in complexity, and if the break in symmetry cannot be spontaneous but induced *outside* of the system, than the complexity leading to evolution is not possible in an *isolated* environment. Some recent investigations have proposed that the break in symmetry which has initiated the processes of the formation of life origins from the impact of the chiral material from the space. The excess of the L forms of amino acids has been found in some meteorites, and most of the scientists agree that their origin is extraterrestrial [10].

One of the specific breaks in symmetry which is crucial for the emergence and the development of life is the appearance of *helical forms* of macromolecules such as polypeptides and nucleic acids. The characteristics of the helical forms is that they are chiral spirals. Such spirals can have either left-handed or right-handed symmetry of helices. In the nature, the prevalent is the right-handed form. Since

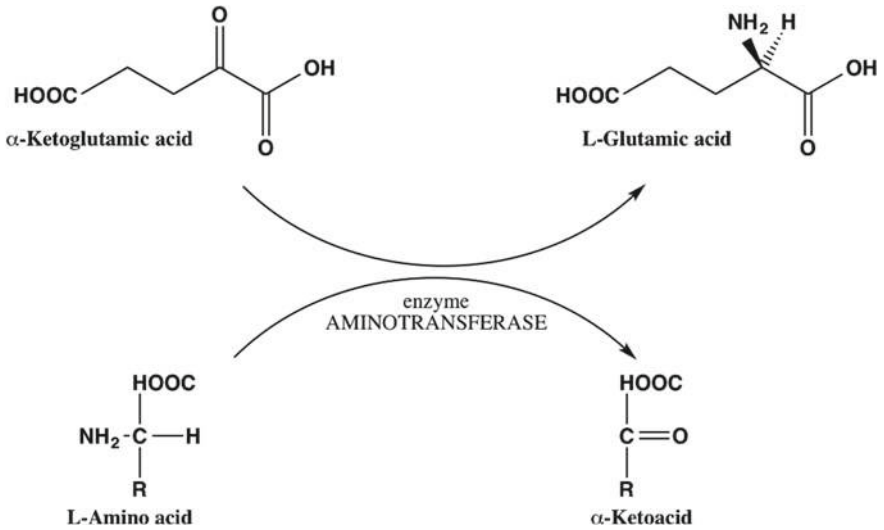


Fig. 2.7 Appearance of the chiral molecule (L-Glutamine acid) in living system in the reaction with the specific enzyme catalyst *Aminotransferaze*

DNA or RNA molecules are the bearers of the hereditary properties, their replications should preserve the original right-handed symmetry. By copying the spiral point by point, the helical symmetry of DNA is preserved (Fig. 2.8). Symmetry break, which have resulted with the appearance of the helical chirality was in the chemical-biological evolution decisive for the emergency of life. The arguments for these facts are provided from the studies of artificial polynucleotide molecules which have disrupted helical symmetry. The possibility of non-helical DNA has been studied by syntheses of polynucleotides with different derivatives of nucleotide monomers. From these experiments it follows that the helical shape of the DNA molecule is consequence of the structure of the nucleotides from which DNA is formed. In the natural DNA the sugar component of the nucleotide is deoxyribose. The artificial DNA molecule in which the sugar component deoxyribose is in nucleotides replaced with glucose, the *homo-DNA* (Fig. 2.9), consists of almost parallel chains of nucleotides (Figs 2.9 and 2.10.), and its right-handed chirality that is essential for the emergence of life is lost [11–13].

As I have just demonstrated in the discussion about the examples of the role of symmetry, the examinations about complexity are especially focused on the problem of the appearance of life followed with the biological evolution. The basic question in these studies is whether the evolution of organisms leads to higher complexity, or the appearance of complexity in evolution is only an epiphenomenon. The theory of evolution is based on the observations of mutational variance coupled with selections. If the mutation and the selection provoke the increase in the diversity of organisms, the another question that appear is whether and how this diversity is correlated with complexity. The largest part of this book is focused on this question.

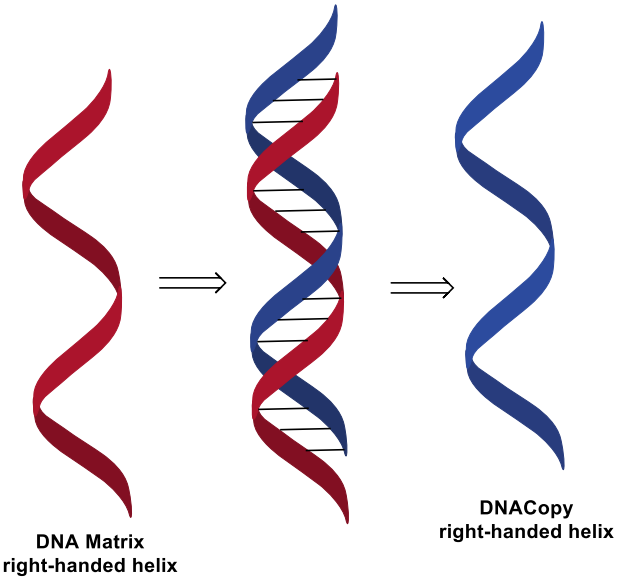


Fig. 2.8 Conservation of the right-handed helix in copying the right-handed DNA matrix. (DNA matrix is in red, and its copy is in blue)

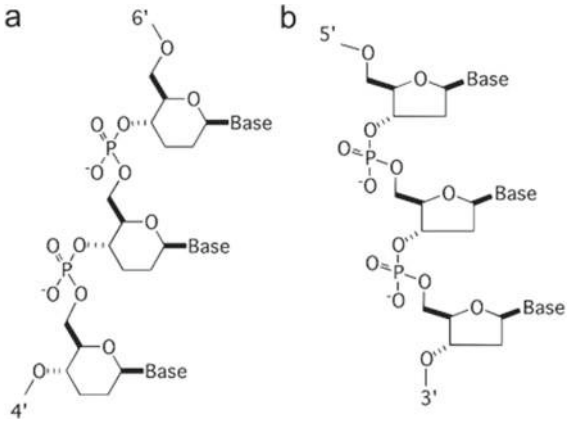


Fig. 2.9 Fragment of the structure of **a** homo-DNA with glucose, and **b** natural DNA with deoxyribose

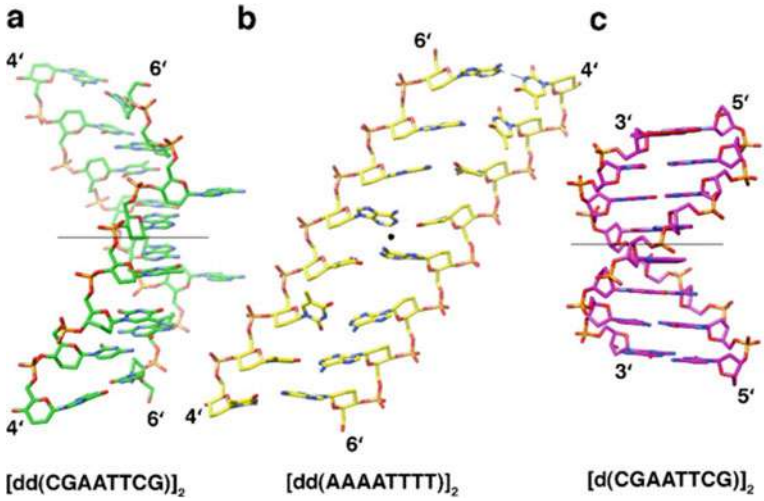


Fig. 2.10 **a, b** Configuration of synthetic homo-DNA, and **c** natural DNA (Reproduced by permission from ref. [13])

References

1. Horgan J (1997) The end of science (Note 11). Broadway Books, New York, p 203
2. Briggs K (1987) Simple experiments in chaotic dynamics. Am J Phys 55:1083–1089
3. Hudson JL, Mankin JC (1981) Chaos in the Belousov-Zhabotinskii reaction. J Chem Phys 74(11):6171–6177
4. Dearden JC (2016) The history and development of quantitative structure-activity relationship. Int J Quant Struct-Prop Relation 1:44
5. Oppenheim P, Putnam H (1958) Unity of science as a working hypothesis. In: Feigl H, Scriven M, Maxwell G (eds) Minnesota studies in the philosophy of science, vol 2. University of Minnesota Press, Minneapolis, pp 3–36
6. Weisskopf VF (1966) Knowledge and wonder: the natural world as man knows it. Doubleday, Garden City, New York
7. Anderson PW (1972) More is different. Science 177(4047):393–396
8. Potochnik A, McGill B (2012) The limitations of hierarchical organization. Philos Sci 79:120–140
9. Humphreys P (2014) Explanation as condition satisfaction. Philos Sci 81:1103–1116
10. Engel MH, Macko SA (1997) Isotopic evidence for extraterrestrial non-racemic amino acids in the Murchison meteorite. Nature 389:265–268
11. Egli M, Pallan P, Pattanayek R, Wilds CJ, Lubini P, Minasov G, Dobler M, Leuman CJ, Eschenmoser A (2006) Crystal structure of homo-DNA and natures choice of pentose over hexose in the genetic system. J Am Chem Soc 128:10847–10856
12. Eschenmoser A (2014) Chemical etiology of nucleic acid structure. Science 284:2118–2124
13. Sheehan JH, Smith JA, Pallan PS, Lybrand TP, Egli M (2019) Molecular dynamics simulation of homo-DNA: the role of crystal packing in duplex conformation jonathan. Crystals 9:532–546

Chapter 3
System Theory

Theory of systems has appeared in the middle of the last century as an attempt to develop a sort of the universal science that could formulate the concepts which are *isomorphic* with the laws of particular scientific disciplines. This theory has been formulated by Karl Ludwig von Bertalanffy who intended to develop the theory that consists of general principles and laws that can be transferred through wide spectrum of scientific fields, a sort of trans-disciplinary science [1]. Principal ideas about the universality of sciences have appeared early in the history of philosophy and art. General and universal science has been in the focus of the philosophies of Plato, Aristoteles, and, later, in the works of thinkers such as Johannes Scotus Eriugena, Raimundus Lullus, Giordano Bruno or Nicolaus Cusanus. Interestingly, the work of art which has inspired the thoughts of Bertalanffy is the literary work of Hermann Hesse "Das Glasperlenspiel" [2] in which the author imagine the society of intellectuals in search for the synthesis of all the sciences and art by using the isomorphic artificial symbolic language.

Bertalanffy's theory is focused to the identification of the holistic dynamic systems, which behave as a whole, and which are formed as a consequence of the pressure of the environment. The basic idea is that a system is more than the sum of its components. As we will discuss later in this book, the behaviour of systems is to some extent independent on the properties of its parts. The formation of systems is a consequence of the iterative bottom-up processes. Consequently, the best method for modelling systems is the application of computer simulations [3, 4]. Systems appear in many fields of research, especially in biology, chemistry as well as in particular social sciences. Special focus of the system theory is to the technology that has been developed after the development of cybernetics [5]. The main principle in cybernetics is the feedback action which regulates the technical automata. For instance, the simple cybernetic system is a thermostat that regulates the constant temperature by feedback effect of the thermometer on the intensity of heating. Bertalanffy has recognized the isomorphic analogy between feedback effect in cybernetics automata and in the biological and biochemical systems. The example of such a biochemical

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system are enzyme catalysed reactions, in which the concentration of the product, if it reaches some critical threshold, inhibits the catalytic activity of the enzyme. In the nature, if living organisms are exposed to the constant changes of the environment, they react on the way to preserve their internal stability by a self-regulating process known as *homeostasis*. Thus, one of the most pronounced properties of systems is their robustness. For instance, one of the most investigated ecological systems, the predator–prey model which is known as the Lotka-Volterra oscillator has been found to be highly robust [6]. Components which can form the system can also be systems, say, the sub-systems. In the nature, as well as in the human organizations the systems can appear within the even larger systems forming the hierarchical construction [7].

Systems are in principle teleological, in the sense, that their performance is adjusted to accomplish particular functions, either in the nature or in technology. Systems are holistically dynamical, and their behaviour cannot be explained solely by knowing the properties of all their components. Bertalanffy suggests, that systems behave law-like, and that these laws could be universal, i.e., they could be applied either to living beings, or to complicated social structures such as large companies or financial systems [8] From the deeper insight in the work of Bertalanffy, it could be recognized that the author de facto discusses also the basic principles of the theory of complexity: in the work of Bertalanffy we can find the principles of non-linear dynamics, as well as the principles of the level structure of the nature. The level structure in the system theory appears in the form of the localization of the system to subsystems with the more or less defined subordinated functions. Evidently, Bertalanffy does not intend to distinguish between the categories of complexity and the categories of the system theory, and how they are interrelated. This is in the focus of this work.

Both, “thinking in systems” and “thinking in complexity” are unavoidable in contemporary science and technology. Last developments in the theory of evolution has evolved from the applied system theory. Manfred Eigen has explained the process of evolution by analysing the emergence of biological information through self-organization. Together with Peter Schuster, Eigen has proposed the *theory of hypercycles* in the self-replicating molecules (for instance, RNA or DNA) which have, hypothetically, appeared on the primordial Earth [9, 10]. Hypercycles are systems of different chemical autocatalytic cycles that compete between each other, and which, under the specific circumstances, could activate the evolutive processes [11].

In chemistry, the importance of system theory became more pronounced mostly in the last decade. It is focused on studies of compartmentalization in supramolecular assemblies, reaction networks, oscillating and switching reactions, autocatalytic systems, self-assembling, and, especially, in prebiotic chemistry [12]. Consequently, the theory of systems plays also the important role in the development of the methods of the “synthesis of life”. The possible precursors of life in the "primordial soup" appear in the form of the chemical compartments with micellar structure. Micelles are aggregates of molecules that form the supramolecular structure characterized with the cavity which is large enough to encompass an ensemble of smaller molecules. Because these molecules appear in such a closed natural vessel, they can in principle be interconverted with each other by chemical reactions. In such a way, the

closed chemical systems which could interact with their environment can be formed. Such supramolecular compartments can also encompass not only the molecules, but also the smaller micelles, forming in such a way the complicated hierarchical structures. Similar compartment formations are in the prebiotic chemistry studies used as the models for the precursors of living cells [13]. In addition, chemists are able to construct also the self-replicating systems that are alternative to the real biological behaviour [14]. Such alternative models must satisfy the basic requirements for the appearance of life: metabolism, self-replication, evolution, and compartmentalization. Such approach is highly important for the understanding of the real natural chemistry which have preceded the biological evolution.

The *problem of function* is of huge interest in modern science, especially in the studies in which chemistry, biochemistry, and biology are overlapped. This problem appears in the form of the investigation of the structure-function relationship of complicated molecules or supramolecular structures. For instance, the enzyme molecule is characterized with its corresponding *catalytic function*, and this function can be operative only if the molecule possesses specific three-dimensional and chiral structure. However, the structure alone, which in many cases could be designed by the methods of chemical synthesis, does not prejudice any function. The *function* of this structured molecule is not in the focus of chemical synthesis, because the chemical synthesis is preoccupied with the development of the methods for the formation of particular molecular structure. Function may have a sense only from the viewpoint of the higher level of complexity–to the *purpose* that is defined within the biological principles. Thus, the biological requirements define the functions of the entity (the molecule) formed on the lower, chemical level of complexity. In other words, biological wholes are holistic systems that define the *role* of the structure of the enzyme molecule. This is manifested as the selective pressure "from the outside" which delineates the nature of the function. In the broader sense, the environment generates the pressure from outside, which is one of the principal driving forces that regulate evolution.

References

1. von Bertalanffy KL (1969) General system theory. G. Braziller, New York
2. Hesse H (1943) Das glasperlenspiel. Fretz & Wasmuth, Zürich
3. Bedau MA (2014) Testing bottom-up models of complex citation networks. Philos Sci 81:1131–1143
4. Wolfram S (2022) Wolfram language documentation. Wolfram Research Inc
5. Wiener N (1948) Cybernetics. John Wiley & Sons, New York
6. Weisberg M, Reisman K (2008) The Robust Volterra principle. Philos Sci 75:106–131
7. Simon HA (1999) The sciences of the artificial. The MIT Press, Cambridge, Massachusetts, p 128
8. Kuhlmann M (2014) Explaining financial markets in terms of complex systems. Philos Sci 81:1117–1130
9. Eigen M (1971) Selforganization of matter and the evolution of biological macromolecules. Naturwissenschaften 58(10):465–523

10. Eigen M, Schuster P (1982) Stages of emerging life—five principles of early organization. J Mol Evol 19(1):47–61
11. Szostak N, Wasik S, Blazewicz J (2016) Hypercycle. PLoS Comput Biol 12(4):e1004853
12. Grzybowski B, Otto S, Philp D (2014) Systems chemistry: a web themed issue. Chem Commun 50:14924
13. Ivanov T, Cao S, Doan-Nguyen TP, Madalosso HB, da Silva LC, Landfester K (2023) Assembly of multi-compartment cell mimics by droplet-based microfluidics. ChemSystemsChem e202300034
14. Otto S (2022) An approach to the De Novo synthesis of life. Acc Chem Res 55:145–155

Chapter 4
Categories of Complexity

The central question in the studies about complexity is how to define and, perhaps, how to measure this property. The first step in the discussion about this question requires the development of the method for the classification of different sorts of complexity. By looking in the literature, especially in the works about the mathematical and the computer sciences, we can find a long list of the definitions of complexity. Some examples were already reviewed [1]. However, in this work I am trying to simplify the classification of complexity dividing it in the three categories: synchronic, diachronic, and combinatorial complexity.

4.1 Synchronic Complexity

The term *synchronic complexity* (*structural complexity*) stands for the complexity of the structures which exist as stable forms close to the thermodynamic equilibrium within a shorter or longer period of time. The idea, that synchronic complexity is structured in levels, origins from the studies about the structural forms of elemental entities and their combinations [2]. The structures of the actual objects can be arranged in different levels, such as atomic, molecular, supramolecular, biological, etc. The relationship between the properties of the higher level structures and the properties of their lower-level components is one of the central questions of mereology [3]. The important elements of such interpretation include primarily the *holistic view*, i.e., the opinion that the structures on the higher level possess the new *emergent* properties. Such properties cannot be explained only by summarizing the properties of the constituents, which belong to the lower level. For instance, water has emergent properties characteristic for the molecular level of complexity, which cannot be extrapolated from the properties neither of hydrogen nor of oxygen. Or, more generally, the properties of the living organisms are emergent in the relation to the properties of the molecules from which the living being consist. In contrary, from the

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reductionistic view there are no emergent properties at all [4]. Instead, the items on some complexity level only interact with each other. However, the consequence of such an argument is the *reduction ad absurdum*: if the properties of the subjects on every level are exclusively the interactions of the particles which are on the immediate sublevel, then this principle can be continued to lower and lower levels ad infinitum. What remains, are only the interactions! As we will discuss here, the transition from the lower to the higher level requires the passage through the so called transition state. The formation of such transition state is possible only if an additional energy is added. In chemistry, this is known as the *activation energy*.

The idea about the authenticity of special sciences is, in principle, based on such level-like structure of complexity. Basic subjects that are in the focus of the special scientific disciplines (say, atoms, molecules, living beings, etc.) are those which have the emergent properties characteristic for the corresponding level of complexity. Consequently, the epistemology of special scientific disciplines should be based on the heuristic assumptions which are formulated starting from corresponding emergent phenomena. This could be a convenient explanation why science consists of special disciplines such as physics, chemistry, biology, etc. [5]. The example for such epistemological authenticity of sciences is the formulation of the specific laws and rules. For instance, the chemical laws about the reaction mechanisms cannot be inductively constructed from quantum mechanical laws. However, the laws formulated on the more basic (lower) level are hierarchically higher: the laws of the science on the higher level of complexity cannot be *in contrast to the laws of the science on the lower level*. The concepts that contradict basic physical laws cannot be accepted as the rigorous scientific concepts.

The mode of sorting of various material subjects in particular complexity levels requires the use of the convenient criteria of classification. One of the possibilities is the use of the interaction energy for mutual bonding of the particles of lower level to form the particles on the higher complexity level [6, 7].

Suppose, that two entities on the lower complexity level unify in the new structure that belongs to the higher complexity level. On the sub-atomic level, association of nucleons, say, protons and neutrons in the formation of corresponding atomic nucleus results with the release of large amount of energy (in common words, nuclear energy), because the higher complexity structure is an atom (the atomic nucleus consisting from protons and neutrons) which is much more stable than the separated nucleons.

In the formation of the structures on the molecular level, two atoms are associated forming the molecule. The consequence of the formation of molecules is, again, the decrease in total energy of the system because the two-atomic molecule always possesses less energy than the sum of energies of two isolated atoms. This energy difference is known as the energy of chemical bond.

The next level is composed from the supra- or super molecular structures, the molecular aggregates which are formed by the non-covalent interaction between the molecules. The stabilization of such structures follows from the loss of energy during formations of these higher-level structures (hydrogen bond energy, van der Waals interactions, halogen-halogen interactions, dipole–dipole interactions, etc.).

In summary, starting from the lowest complexity level, for instance from elemental particles, then following with atomic level, then molecules and molecular aggregates, etc., each transition to the higher complexity level requires corresponding energies of interaction between entities. Some representative interaction energies required for the transition from lower to the higher complexity levels are represented in Table 4.1 and in Fig. 4.1.

The relations represented in the Fig. 4.1 reveal that the interaction energy for the formation of atoms from elemental particles is by 10^7 orders of magnitude larger than the chemical bond energy. In going to the next higher complexity level where the supramolecular structures are formed, the energy of aggregation of molecules by hydrogen bond is only five-fold lower than the chemical bond energy, and van der Waals binding the energy of molecules in liquids or in molecular crystal is still much lower, almost negligible. From the relationship between the energies of interactions and corresponding complexity levels shown on the Fig. 4.1, the two asymptotic limits can be recognized. On the right side of the diagram, how the structural (synchronic) *complexity grows*, the *energy of interactions* required for the formation of higher complexity levels *diminishes* asymptotically approaching to zero. Thus, it is not possible to enhance the structural complexity ad infinitum because the interaction energy becomes infinitesimally low and the stable more complex structures cannot

Table 4.1 Interaction energies for the formation of the entities on the different levels of complexity (adapted from [5])

Interaction (level of complexity)	Example	Energy in $kJmol^{-1}$
Nuclear	$2^1H + 2n \rightarrow {}^4He$	2.7×10^9
Chemical	Bond energy of H_2 molecule	435.5
Supramolecular	Hydrogen bond	20
Intermolecular van der Waals	Interaction between two CH4 molecules separated by 3.8 Å	2.5

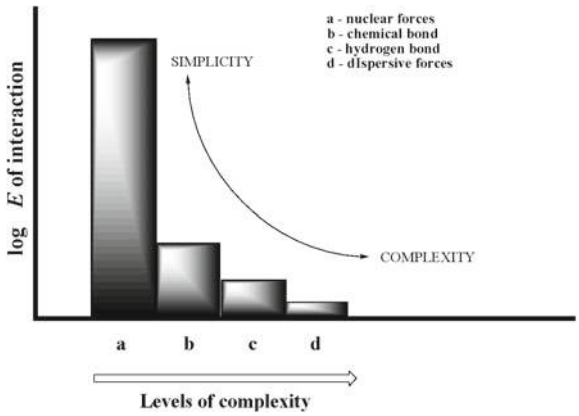


Fig. 4.1 Complexity classified in the levels *versus* the logarithms of the energy of interaction of particles (atomic nuclei, molecules, and molecular aggregates…) to form entities on the higher level (Reproduced by permission from [7])

be formed. This principle has been called the *principle of diminishing interactions* [5].

On the left side of the diagram on the Fig. 4.1, the *increase in simplicity* is followed with the growth of the interaction energy. Since the absolute simplicity would require infinitesimally high interaction energy, it cannot be reached. Accordingly, *absolute synchronic simplicity and absolute synchronic complexity are not possible*. Thus, we could conclude that the synchronic complexity is constrained by the instability of structures. The level of complexity which is in the focus of the investigations within chemistry, where molecules and molecular aggregates are formed, is situated in the middle of this diagram – chemistry is the central science!

4.2 Diachronic Complexity

Historically, the science about diachronic complexity has been formulated gradually, perhaps during the development of the science about the motions of planets within the solar system. The so-called three-body problem in the Newtonian mechanics, as well as its extension to the mechanics of many-body systems, have motivated the appearance of the idea about the complex system problem. The clearly formulated concept about the open irregular/regular behaviour of mechanical systems can be found already in the work of Henry Poincare [8]. Later this problem has been formulated as the KAM theorem (Kolmogorov, Arnold, Moser) [9]: the solar system is, in the same time regular and irregular, and it could be under particular conditions chaotic. This "position" of the solar system between chaos and regularity is the example of the maximum of complexity. In the popular literature, the theory of diachronic complexity is frequently identified with the theory of chaos.

The theory of diachronic complexity is transdisciplinary, because their main principles are the same in the wide spectrum of scientific fields. It appears, for instance, in chemistry, especially after the discovery of the oscillatory reactions such as the Belousov-Zhabotinski oscillator [10], or in biology within the Lotka-Voltera discoveries of oscillations in the ecological systems [11, 12]. It is widely used also in economy and management by studying the behaviour of the complex social systems [13]. As I have already mentioned, in the middle of the last century, von Bertalanffy applied the principles of chaos theory as a basis for his more general *theory of systems*.

Belousov-Zhabotinsky reaction system is probably the most investigated one. These coupled reactions appear in the mixture of malonic acid, bromate, strong acid (for instance sulfuric acid), and the metal ion catalyst. The reactions are monitored by observations of the changes of colour caused by different ratios of oxidized and reduced forms of the metal catalyst. If the reaction conditions are fine-tuned, the solution of these reactants starts to change its colour periodically indicating the periodic change of the oxidized catalyst. The tuning of the reaction conditions can include, for instance, the change of temperature, the variation of the specific irradiation of the reaction vessel, etc. In the experiment where the reaction occurs in the photosensitive

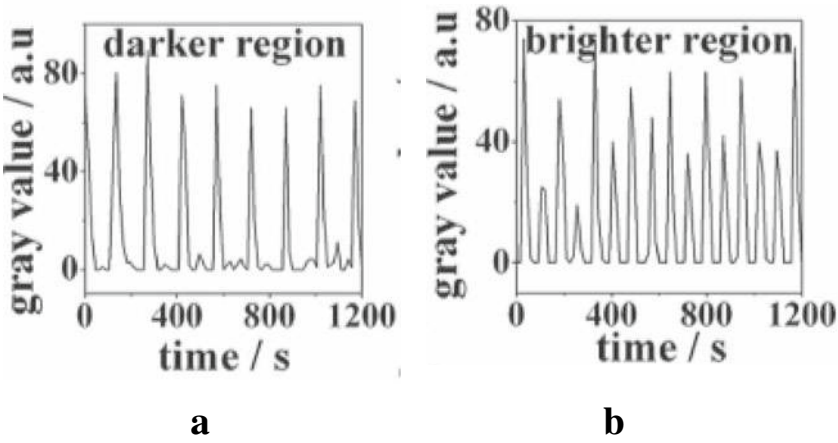


Fig. 4.2 Photo-sensitive oscillating reactions which differ in the diachronic complexity: **a** almost regular in the dark, and, **b** chaotic after irradiation (Reproduced by permission from [14])

gels, the oscillations of the reactions are either almost regular or chaotic (Fig. 4.2a, and b), depending whether the reactor is irradiated or not [14].

In biochemistry, one of the most important reaction systems in organisms is the redox system that is known as the citric acid cycle (Fig. 4.3). Variation of its diachronic complexity could cause serious damage of the living system.

Historically, Belousov's studies were primarily focused on the problem of the kinetic analysis of the citric acid cycle. Since, at the time, this reaction system was too complicated to be studied experimentally, Belousov has designed the simpler reaction system that has served as a model for the citric acid cycle. Today, the oscillatory behaviour of citric acid cycles was studied directly in biological cell organelles such as in the mitochondria [15]. For instance, oscillations of Ca^+ ion indirectly caused by citric acid cycle oscillations represents the convenient example for explaining the variations in diachronic complexity (Fig. 4.4). The lowest diachronic complexity appears as regular oscillations, such as oscillations of Ca^+ ion in Fig. 4.4a. Oscillations of histamine (one of the components in this reaction cycle) observed as the change in intensity of the fluorescence signal afford either some irregularity (Fig. 4.4b), or complete irregularity (Fig. 4.4c). Chemical oscillators can be extremely complex, especially in the living systems. Computer modelling of the system with more coupled chemical oscillators shows that the oscillating circles can be synchronized [16]. Such a synchronization probably appear in organisms and it perhaps takes an important role in the pre-biological evolution on the boundary of life.

The chemical oscillators, regarded as systems, can be decomposed into individual microprocesses. Every of these microprocesses is characterized with corresponding rate. In chemical kinetics, the parameter "rates of chemical reactions" are replaced with the "rate coefficients" (in some cases the term "rate constant" is used) because the rates depend on the concentration of the substance which is changing during the

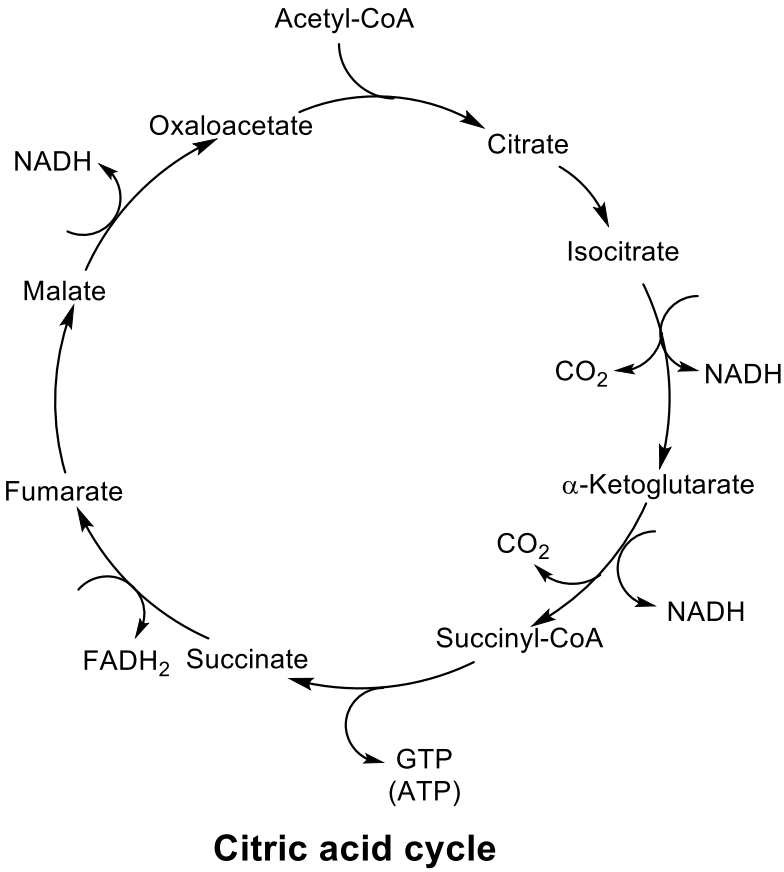


Fig. 4.3 Diachronic complexity of the biochemical cyclic system

passage of time. In contrast, the rate coefficients do not depend on the concentration, and they are characteristics of particular chemical reactions. The rate coefficients of the microprocesses whose combination forms the chemical oscillator should be concerted in particular way. The ratios of these rate coefficients of all the microprocesses are critical for the formation of the stable chemical oscillator, the system. This fact is crucial for the transition of chemical to biological evolution. The evolution can begin only if this sort of diachronic complexity reaches its maximum. That means that the diachronic complexity also converges to some limit. In this limit, i.e., in the maximum of the diachronic complexity, the range in which rate coefficients appear should be relatively narrow. Since the rate coefficients depend on the temperature, this is possible only within the narrow range of temperatures. In the extreme conditions, in the environments where the temperatures diverge substantially the diversity of different reaction rates is enormous, and the state is chaotic. On the other side, if

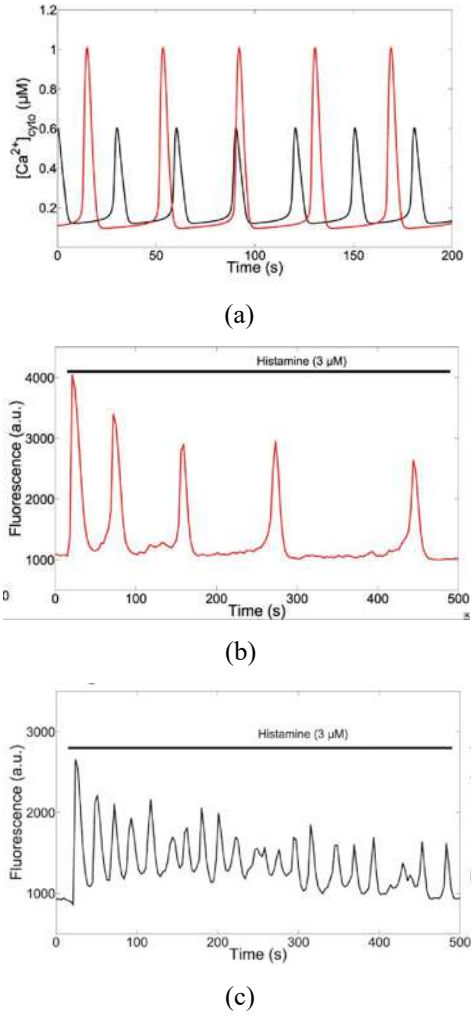


Fig. 4.4 Chemical reaction oscillations observed in the modelling of the citric acid cycle in the cell mitochondria. **a** regular oscillations with the low complexity; **b** more complex oscillations with some degree of irregularity; **c** chaotic highly complex oscillations (Reproduced by permission from [15])

the temperature is spanned within too narrow scale, the number of various processes is too small to form the stable oscillating system.

Regulation of the ratios of the reaction coefficients appears in the nature also as an effect of the enzyme catalysts. In the Fig. 4.5 are represented the rate coefficients for the hydrolytic reactions in the case when they are non-catalysed, and in the presence of the catalyst. While the non-catalysed rate coefficients are spanned in the wide range between $10^{-1}s^{-1}$ and $10^{-15}s^{-1}$, the catalysed reactions appear between much narrower scale (10^{-1} – 10^{-8} s^{-1}) [7, 17]. Within this narrow range can appear the maximum of diachronic complexity.

Chemical autocatalytic systems such as Belousov-Zhabotinski oscillator can also be used for designing a sort of chemical computer. The advance of this computer is

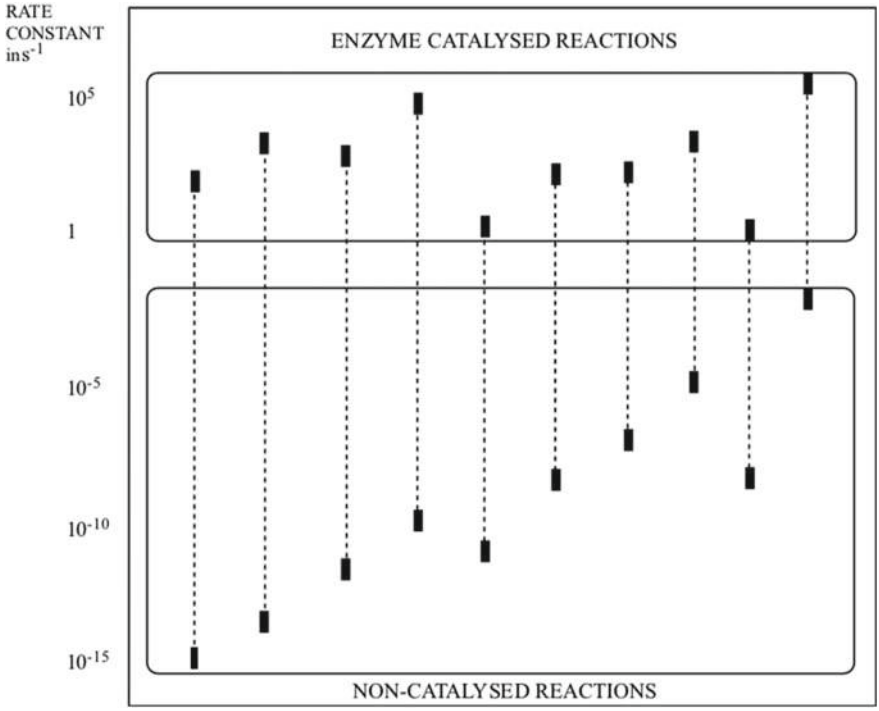


Fig. 4.5 The range of the reaction coefficients of enzyme catalysed and non-catalysed hydrolytic reactions. Reproduced by permission (Reproduced by permission from [17])

that it avoids the so called von Neumann bottleneck, which constrains the communication between memory and processing. All modern computers are based on the silicon chips and in their architecture the memory and processing units are separated. First experiments in the field of chemical computers which are structured from a series of cells with individual partially interconnected Belousov-Zhabotinski oscillators show the possibility of computing in original way [18].

4.3 Combinatorial Complexity and Entropy

Almost within the same historical period when the ideas of synchronic and diachronic complexity have appeared, the concept of complexity has been developed within computer science, logics, theory of automata, linguistics, and in some special mathematical disciplines. In computer science, the term complexity has been introduced in relation with the form and the size of computer programs. Andrey Kolmogorov, and, independently, Gregory Chaitin and Ray Solomonoff, have defined complexity as the size of the minimal computer program that can represent the item, or, the size

of the minimal program whose output completely describes this entity [19, 20]. For instance, if the entity is a repetitive pattern with the translational symmetry, then the program which represents it is relatively simple. However, the entities can be so complex, that the program which represents them is of the same size as the interpreted entity.

Almost ideal model for the Kolmogorov complexity can be found in the construction of constitutional formulas in chemistry, especially in organic chemistry. Chemical formulas are represented as topological objects that could be visualized in the form of graphs in two dimensions. Representation of graphs [21] by using the so-called neighbourhood matrices with their corresponding determinants is an example of Kolmogorov complexity. The basic principles of the graph theory will be discussed in the next chapter. Chemical formulas and their interpretation by using chemical nomenclature is a good example for explaining Kolmogorov complexity. As it is shown in the Fig. 4.6, the repetitive structure of the *undecane* molecule has low complexity because its representation (its chemical formula) is simple, such as $(CH_3(CH_2)_9CH_3$. On the other hand, the complexity of the steroid molecule, represented on the bottom of the Fig. 4.6, is maximal since the representation is of the same size of complexity as it is the interpreted structure. Let us call this kind of complexity the *combinatorial complexity*.

The complexity of the molecular as well as the complexity of the biological morphological structures represented in the three-coordinated space has been studied

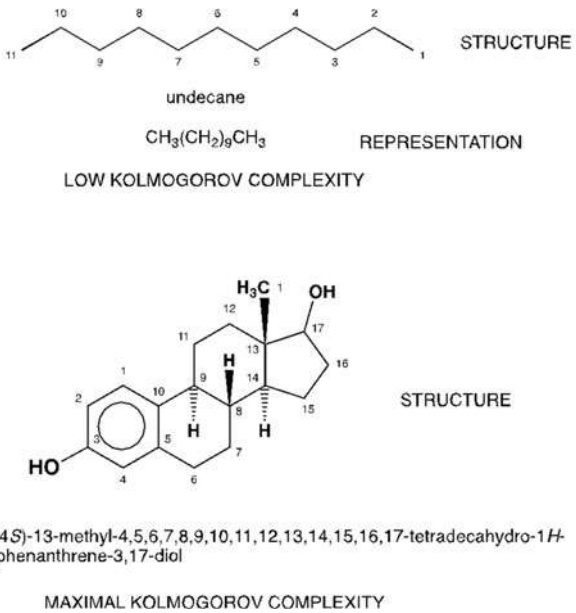


Fig. 4.6 Kolmogorov-like complexities of chemical structures. While the representation of the upper structure is much simpler than the structure, the representation of the structure on the bottom is of the same complexity as it is the structure itself

by a proposing a sort of coding principles [22]. The special focus in this research was on the relationship between the regularity and complexity. In this study molecules and biological components are discussed as the examples of the structural complexity. However, in the frame of the terminology of this book, this research should belong to the combinatorial complexity.

The increase in the combinatorial complexity is possible only by the addition of some new information from the outside. This new information appears in the form of the impact of particular limitations imposed to the rules used for the formation of the structures, or the limitations imposed to the laws of physics or chemistry [23]. For instance, in the graphs representing chemical formulas, the limitation is the introduction valency: points representing the carbon atoms have only four valences, i.e., they can be connected maximally with four neighbouring points. How I will demonstrate later, this idea looks like a paradox because although such limitation reduces the diversity of structures and the freedom of their formation, it still increases complexity.

Molecular graphs which represent the constitution of molecules are topological objects, i.e., they are invariant on the nature of the space. The mathematical manipulation with molecular graphs in the quantification of combinatorial complexity is traditionally used in chemistry [24]. As it has been already mentioned, to obtain the higher complexity level, the introduction of *new information* is necessary. In the chemical structural theory, the new information is also the introduction of the Cartesian three-dimensional space with the consequence that molecules assume configuration, i.e., their spatial shape and chirality. Spatial configurations that were already discussed in previous chapter is in the heart of stereochemistry, and it plays the most important role in the discussion about the structure-function relationship.

Another approach to the combinatorial complexity has appeared in the *theory of automata* developed by John von Neuman [25]. Von Neumann has investigated the possibility of the spontaneous appearance of complexity. The pictorial form of von Neuman automata can be found in the "new kind of science"-like investigations developed by the computer scientist Stephan Wolfram who has described the development of complex forms by using the progressive growth of the deterministic patterns starting with corresponding simple rules. However, such development of visually complex forms is in principle not the growth of complexity because the developing pattern is completely determined and fixed by the information incorporated in the starting rule. During the stepwise development of pattern there is no effect of any additional external information. Quite oppositely, the Wolfram complexity is in principle the *complexity of the rules* as such (because the rules are the external information), and the complexity of the developing patterns is only the consequence of these rules. The details about the Wolfram's theory of cellular automata will be discussed in Sect. 4.3.4.

In the previous section we have suggested that the synchronic complexity approaches asymptotically to some limit because the interaction energy for the formation of higher aggregates gradually vanishes.

The possible confines in combinatorial complexity I will discuss by studying the relationship between complexity and entropy, or, in another words, between

complexity and diversity. Such an approach is especially important in the development of methods used in the analysis of the large data collections in modelling and inference in a wide spectrum of sciences and technology [26]. Within the frame of the information theory, the entropy, as it has been defined by Claude Shannon, is related to the probability of some arrangement of entities to obtain particular configuration [27]. For example, if the entity is a coin, the probability that it will fall on each of sides is ½. The entropy of this system can be calculated by using the Shannon formula, where H is Shannon entropy, and $p(x_i)$ is the probability that the coin falls on the particular side (1/2). If there are two coins, $n = 2$, and the calculated entropy is equal –0.693:

$$H(X) = -\sum_{i=1}^{n} p(x_i) \ \ln \ p(x_i)$$

$$H(X) = -\sum_{i=1}^{2} 1/2 \ \ln \ 1/2$$

$$H(X) = 0.6931$$

Since any configuration can be situated somewhere between the limits of order and disorder, the information theory enables us to calculate the correlation of the Shannon entropy and complexity. Interestingly, the maximal complexity does not match the maximum value of entropy, i.e., the maximal value of diversity. Rather, the highest complexity has its maximum at some value of entropy that is closer to order than to the disorder limit (Fig. 4.7) [28].

Another approach to the explanation of the combinatorial complexity is nicely described in the book "At home in the universe", by Stuart Kauffman [29]. However, the understanding of this Kauffman's method requires the understanding of the basic principles of graph theory. Accordingly, let me delineate the basic principles of graph theory in more details by using chemical graph theory as a model.

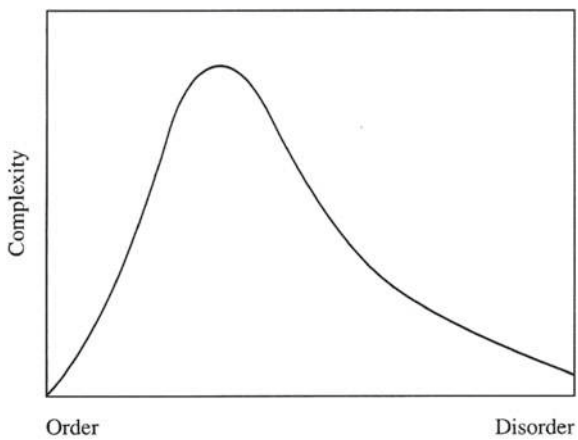


Fig. 4.7 Relationship between the degree of disorder and complexity (Reproduced by permission from [28])

4.3.1 Graph Theory and Topology

During the development of the application of quantum mechanics to chemistry in the middle of the last century, Erich Hückel has demonstrated that the electronic structure of, for instance, benzene molecule could be estimated just by looking on its structural formula, i.e., its graphical representation. This discovery has initiated the studies of the relationship between graphical description of structural chemical formulas and physical and chemical properties of corresponding compounds. Graph theory is the special case of the broader mathematical branch called topology. However, topology has been invented a long time before the appearance of such a chemical graph theory. Let us mention, that the similar graph theory representation has been applied also for the studies of the systems in the vide variety of sciences, for instance, in the research in anthropology [30].

The idea about the science about the connectivity between objects, independently on the nature of the physical space in which they exist, has been invented already in XVIII century. Leonhard Euler has imagined the puzzle which involves the question whether it is possible to pass over all the seven bridges in the German city Königsberg (Fig. 4.8) in such a way that every bridge is passed only once. Neither of the bridges should be skipped. This has been the idea which has initiated the appearance of the at the time new field in mathematics, the topology. Topology is universal. It can be the representation of the connectivity between people in a society as well as the representation of the connectivity between atoms in molecules. To solve the puzzle about the Königsberg bridges, Euler has invented new representation of such topological patterns by using the visualization in which the interconnected objects are described by graphs. Such approach to the topology by using the graph representation is in the heart of the graph theory. Within such description, the system of the Königsberg bridges is illustrated by the graph in Fig. 4.9.

The seven bridges in the Fig. 4.9 are labelled by numbers, and the four lands that are connected by these bridges are labelled by letters **A**, **B**, **C**, and **D**. Thus, this graph, as well as all the graphs, is composed from *vertices* and *edges*. Here we have four vertices (**A**, **B**, **C**, and **D**), and seven edges. Note, that the vertices in the graph differ in the number of edges with which they are connected. For instance, while vertex **A** has five connections (1, 2, 6, 4, and 3), other vertices (**B**, **C**, and **D**) have only three connections (1, 2, and 7 for **B**; 3, 4, and 5 for **C**; and 5, 6, and 7 for **D**). This property of a vertex is called the *valency*. Thus, while the valency of **A** is five, **B**, **C**, and **D**, all have the valency three.

Graphs as the topological objects in which the basic property is the connectivity between the vertices can be mathematically represented by matrices of neighbourhood and by their corresponding determinants. For example, the graph in Fig. 4.9 is represented by matrix in which the diagonal elements are labelled with "x". If the vertices are connected with only one line, the matrix element is equal 1.If two vertices have two connections, the matrix element is equal 2. All the other matrix elements have the value zero (Fig. 4.10).

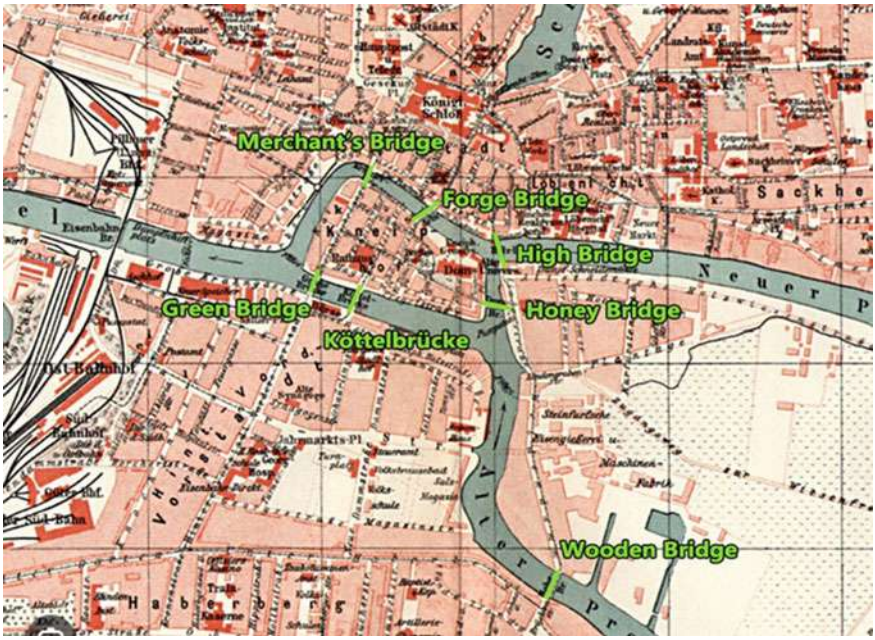


Fig. 4.8 The seven bridges in Königsberg (Wooden bridge, Köttelbrücke, Green Bridge, Merchant's Bridge, Forge Bridge, High Bridge, and Honey Bridge)

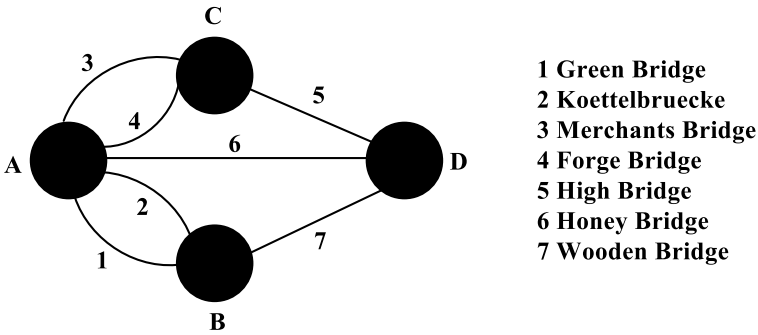


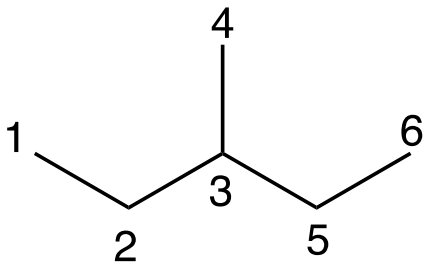
Fig. 4.9 Graph representation of the seven bridges in Königsberg

Another representation of the graph is by means of the *distance matrix*. For its construction let us use the graph in which the vertices are labelled with numbers from 1 to 6:

$$
\begin{array}{c}
 \\ A \\ B \\ C \\ D
\end{array}
\begin{array}{c}
\begin{array}{cccc} A & B & C & D \end{array} \\
\begin{pmatrix}
x & 2 & 2 & 1 \\
2 & x & 0 & 1 \\
2 & 0 & x & 1 \\
1 & 1 & 1 & x
\end{pmatrix}
\end{array}
\qquad
\begin{vmatrix}
x & 2 & 2 & 1 \\
2 & x & 0 & 1 \\
2 & 0 & x & 1 \\
1 & 1 & 1 & x
\end{vmatrix}
$$

Z det Z

Fig. 4.10 Matrix representation of the graph shown in Fig. 4.3.1.2 (Z), and its determinant *det* Z



The matrix elements of the distance matrix represent the number of edges by which the vertices are distant from each other. For instance, the vertex 1 is from the vertex 6 distant by four edges, or, the distance of 4 from 6 is three edges. Consequently, the matrix element for the for the distance 1 to 6 is equal 4, and the matrix element for the distance 4 to 6 is equal 3. The complete matrix has the form:

$$
\begin{array}{c}
 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6
\end{array}
\begin{array}{c}
\begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\
\begin{bmatrix}
0 & 1 & 2 & 3 & 3 & 4 \\
1 & 0 & 1 & 2 & 2 & 3 \\
2 & 1 & 0 & 1 & 1 & 2 \\
3 & 2 & 1 & 0 & 2 & 3 \\
3 & 2 & 1 & 2 & 0 & 1 \\
4 & 3 & 2 & 3 & 1 & 0
\end{bmatrix}
\end{array}
$$

Application of graph theory is especially useful in chemistry. Chemical structural theory and the representations of chemical compounds by structural formulas is in principle a graph theoretical approach: the vertices represent atoms, and the chemical bonds are represented by the edges. This analogy between graphs and chemical

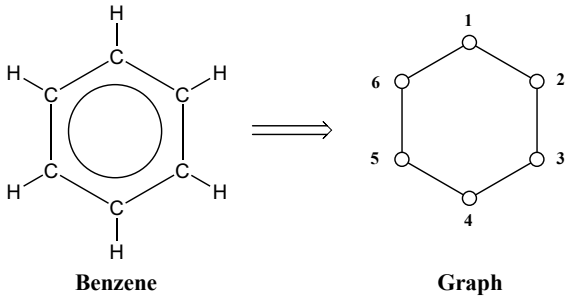
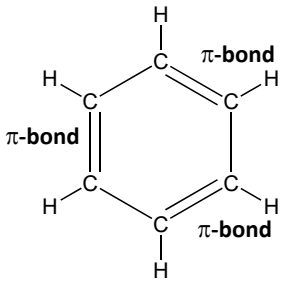


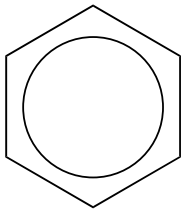
Fig. 4.11 Chemical formula of benzene and its graph-theoretical representation

formulas is shown in the Fig. 4.11. In chemistry this theory has a special name: the *chemical graph theory*.

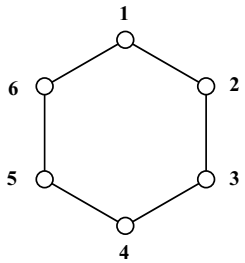
New correlation between graph-theoretical representation and properties of substances has appeared in the year 1930/31 when Erich Hückel has applied quantum mechanics in the study of electronic properties of organic compounds. Hückel has simplified the structure of benzene by looking only the combinations of the double bonds between the carbon atoms (the combination of π-bonds):



As it is known from chemistry, the π-bonds are not localized on the positions as it is represented on the upper scheme. Really, all of the six electrons in π-bonds, the π-electrons, are equally distributed over the complete benzene ring, what is symbolized with the circle within the hexagon.



Thus, represented as a graph, benzene molecule in which only the π-electrons are taken into description is described with the graph:



Graph

The determinant of the matrix representation of this graph has 6 columns and 6 rows:

$$
\begin{array}{c|cccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 \\
1 & x & 1 & 0 & 0 & 0 & 1 \\
2 & 1 & x & 1 & 0 & 0 & 0 \\
3 & 0 & 1 & x & 1 & 0 & 0 \\
4 & 0 & 0 & 1 & x & 1 & 0 \\
5 & 0 & 0 & 0 & 1 & x & 1 \\
6 & 1 & 0 & 0 & 0 & 1 & x
\end{array}
$$

As it is represented, the bonds (edges) exist only between neighbouring vertices (C-atoms). Accordingly, the matrix elements of all the bonds between the neighbouring atoms are labelled with the number 1. All the other atoms are not bound to each other, and the rest of the matrix elements are equal to zero. This determinant can be transformed to the polynomial of the sixth order:

$$x^6 - 6x^4 + 9x - 4 = 0$$

This polynomial is known as the *characteristic polynomial of the graph*. The six solutions of this characteristic polynomial are following:

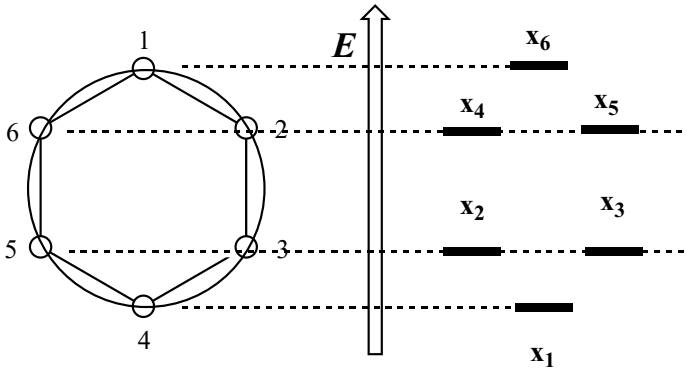
$$x_1 = -2$$

$$x_2,\ x_3 = -1$$

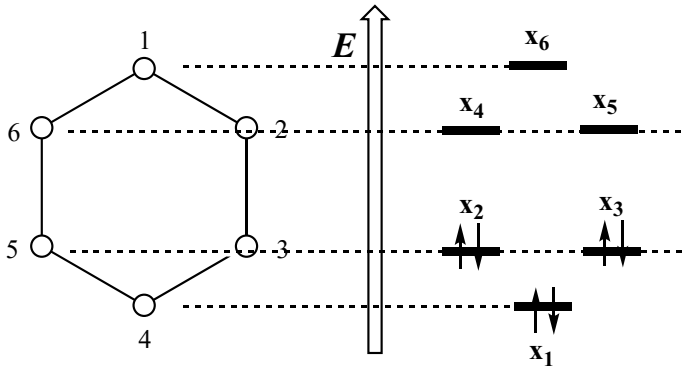
$$x_4,\ x_5, = 1$$

$$x_6 = 2$$

These solutions, $\mathbf{x_i}$, are approximately the energies of all the six π-electrons in the benzene molecule. Hückel has discovered that if the benzene hexagon is inscribed in the circle with the radius r = 1, the same solutions (i.e., the possible π-electron energies, $\mathbf{x_i}$) of the polynomial are equal to the horizontal projections of the vertices:



By occupying these energy levels, the so called π-*molecular orbitals*, with electrons, how it is shown on the following scheme, we achieve the picture of the π-electron distribution in the benzene molecule. Consequently, the molecular graph is directly correlated with the molecular physical properties, in this example with the energies of electrons.



As we have demonstrated, the application of the graph theory is universal. It could be a convenient method for the analysis of various interrelations between objects, independently whether they are atoms or, for example, islands and coast as it is shown on the example of the Köningsberg bridges. Such graph theory can also be helpful in the extension of our concepts about the basic principles of the combinatorial complexity.

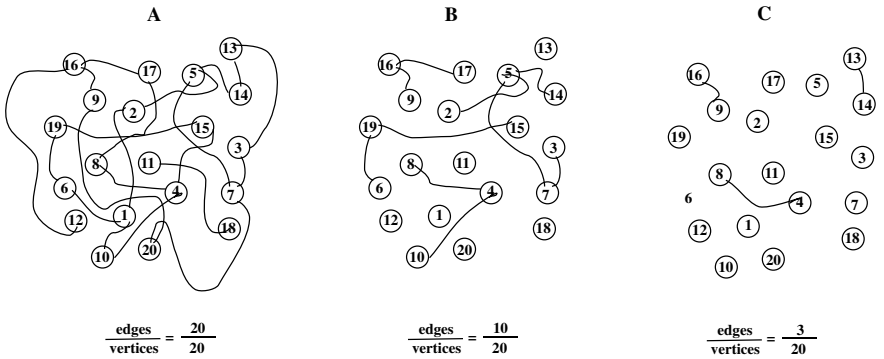


Fig. 4.12 Different phases in the decomposition of the graph consisting from the interconnected 20 elements (accommodated from [29])

The following example, which has been developed by Stuart Kauffman [29], demonstrate how graph-theoretical approach can explain the change in interconnectivity, which could occur, for instance, during the processes such as phase transformation, or polymerization/depolymerization. Imagine, that we have a group of objects which are mutually related in some way, and whose interrelations change in time. The example of such relations can be represented by graphs in Fig. 4.12. The objects are in the Figure labelled with circles, and the connections between them is labelled by lines. The extent to which the circles are interconnected (for instance in going from A to C in the Figure) can be used as a measure of complexity. During the time, the number of new connections between the objects decrease, starting with completely cross-linked collection (**A**) to the almost non-connected group (**C**). Three typical cases of the possible connections between 20 objects are extracted in the Fig. 4.12: the most interrelated objects in the figure A, and the lower levels of interconnectivity in graphs B and C.

By investigating the different levels of the connectivity in A, B, and C in the Fig. 4.12, it could be recognized that in A, all the elements are interconnected. The number of the connected edges (20 elements) and vertices (20 interconnecting lines) is equal. In going to B, and C, the number of edges diminishes and the ratio of edges/vertices is decreasing. Suppose, that we have the large analogous system with thousands of elements. The ratio of edges/vertices in such a large system can be plotted versus the length of the longest interconnecting line that appear during the process of the continuous decrease of the number of the interconnections between the elements. Such a correlation is shown in Fig. 4.13. The curve in Fig. 4.13 is sigmoid, and it is characteristics for the descriptions of phase transitions.

The black point on the curve (Fig. 4.13) is the inflection in which the step-wise shortening of the line, which interconnect the elements, as a function of the edges/vertices ratio is promptest. The sigmoid and its derivation are shown in the Fig. 4.14. The inflection on the sigmoid corresponds to the maximum on the derivation of this function. As we will discuss later, this point is a sort of the "transition state" between

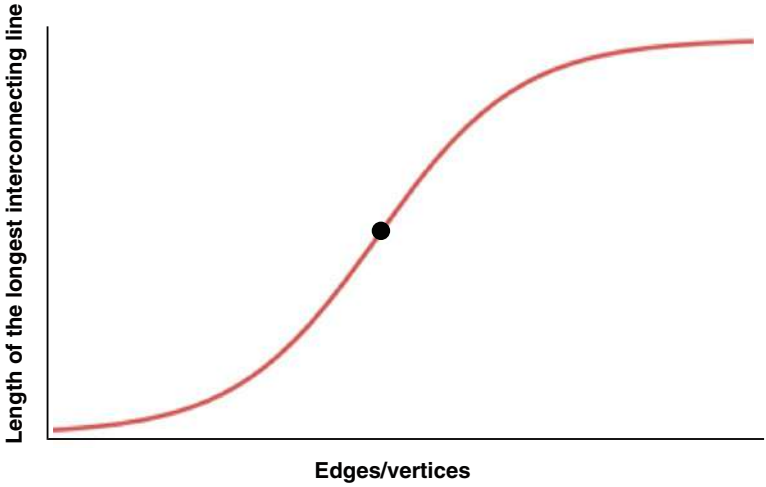


Fig. 4.13 Correlation between the longest interconnecting line and the edges/vertices ratio. The black point is the inflex where the transition state appears

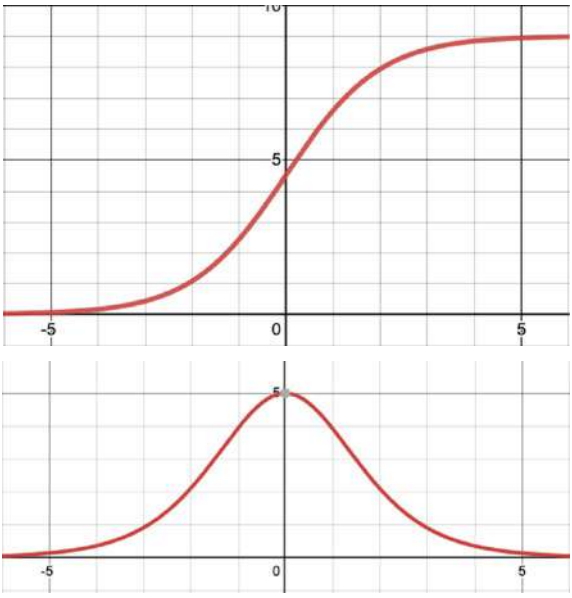


Fig. 4.14 Sigmoidal function (top) and its derivation (bottom)

the simple homogeneity and the chaotic continuum. In this inflex, the combinatorial complexity reaches its maximum.

Since the sigmoidal shape of the curve in Fig. 4.13 is analogous to the curves characteristic for the phase transition, the process of the binding of these elements

from individual units to the totally bound system is a model for such type of transformation. Similar curves can be obtained, for instance, in the processes of melting, evaporation, or autocatalytic chemical reactions.

Now, if we represent the graphs from Fig. 4.12 by the determinants of the adjacency matrices on the way how it is used within the graph theory, the connectivity between 20 objects in the starting connectivity **A** will be represented with the determinant:

$$\begin{vmatrix}
x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & x & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & x & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & x & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & x & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & x & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x
\end{vmatrix}$$

In this 20×20 determinant (because there are 20 objects) the connection between objects is labelled with 1, and if the objects are not interconnected, the matrix element is equal to 0. Trivially, since each object is connected to itself, the diagonal element is labelled with x.

The less interconnected case **B** is represented by the determinant that can be decomposed in four independent block determinants because the rest of the determinant are only zeros:

$$\begin{vmatrix} x_2 & 1 & 0 & 0 & 0 \\ 1 & x_5 & 1 & 1 & 0 \\ 0 & 1 & x_7 & 0 & 1 \\ 0 & 1 & 0 & x_{14} & 0 \\ 0 & 0 & 1 & 0 & x_3 \end{vmatrix} \begin{vmatrix} x_9 & 1 & 0 \\ 1 & x_{16} & 1 \\ 0 & 1 & x_{17} \end{vmatrix} \begin{vmatrix} x_6 & 1 & 0 \\ 1 & x_{19} & 1 \\ 0 & 1 & x_{15} \end{vmatrix} \begin{vmatrix} x_8 & 1 & 0 \\ 1 & x_4 & 1 \\ 0 & 1 & x_{10} \end{vmatrix}$$

$$\begin{bmatrix} x_2 & & &

In chemistry, the principles of the percolation theory can be used as a model for the representation of the chemical process called *step-growth polymerization* [34]. Starting with the model described in the Fig. 4.12 this process can be described in the following way: suppose that 20 elements in the Figure C represent the molecules of monomers, and these monomers polymerize through the transition state (B) to the final polymer (A). This process flows through the complex structure of the "transition state" B that appears between the simplicity C, and the chaotic homogenous state A. It could be imagined that the transition state B appears in the region around the black point (the inflection) on the curve in Fig. 4.13.

The example of such a step-growth mechanism is the polymerization of the nitroso-aromatic monomers in the poly-crystalline phase in which the molecules are pre-oriented in such a way that the nitroso groups which should interact to form new chemical bonds are close to each other (Fig. 4.15).

The kinetics of this process can be easily studied by infrared spectroscopy by looking on the increase in intensity of the signal characteristic for the $^{-}ON^{+} = N^{+}O^{-}$ group of the product polymer. In addition, the disappearance of the starting monomer molecules is simultaneously followed by looking in the decrease of their characteristic signals associated with the functional groups N = O, and C–C (Fig. 4.15).

Independently whether we are analysing the decrease of the starting monomer molecules (Fig. 4.16, blue, and red curves), or we are analysing the appearance of the polymer (Fig. 4.16, black curve), the process is best described with the sigmoid curve. In the inflex points close to the crossing of the curves, the growth of the polymer chains is most pronounced [35]. This point is the state of the maximal combinatorial complexity.

Similar random graph approach has been applied also in the evolutionary biology. The appearance of species in the evolutionary process involves interactions between several different populations. The result of such interactions is the formation of the network of interconnections. In the evolutionary theory this process is called *cohesion* [36]. The network of the cohesion of species can also be represented by graph theory.

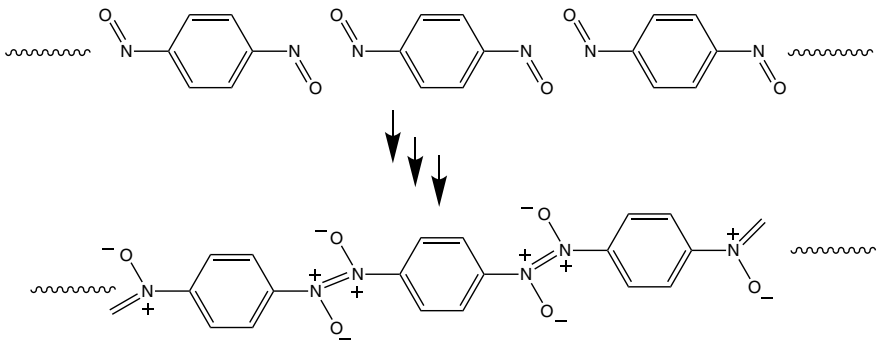


Fig. 4.15 Polymerization of 1,4-dinitrosobenzene (top) to corresponding polymer (bottom)

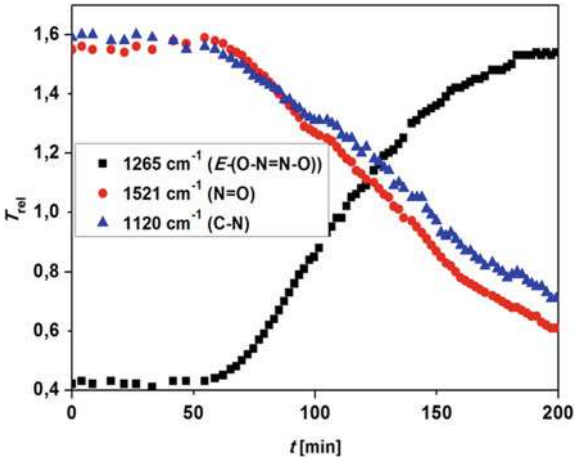


Fig. 4.16 Kinetics of polymerization of 1,4-dinitrosobenzene in crystals. The squares represent the kinetic curve for the appearance of the polymer (characterized by the intensity of the infrared peak of the polymeric O-N = N–O group). Circles and triangles are kinetic curves of the disappearance of the monomer molecules (characterized by diminishing of the monomer signals of the N = O and C-N groups) (Reproduced by permission from [35])

It is illustrated in the Fig. 4.17 where the species in the graph are labelled with the vertices, and their connections are represented by the edges.

The cohesion structure which is shown in the Fig. 4.17 can be discussed in the frame of the combinatorial complexity. Accordingly, the Shannon entropy for this graph is possible to calculate by using the equation which has been explained earlier in this chapter. Its value is 1.5867.

$$H(X) = -\sum_{i=1}^{n} p(x_i)\ \ln\ p(x_i)$$

$$H(X) = -[(2)(3/12\ln 3/12) - (3)(2/12\ \ln\ 2/12)]$$

$$H(X) = 1,5867$$

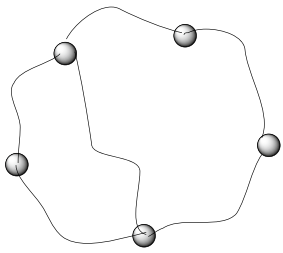


Fig. 4.17 Graph representation of the cohesion of 5 species (labelled with the vertices)

Now, let me extend the example of the cohesion of species to the collection of 14 entities that interact between each other to form the network. The decrease in the connectivity between these 14 species (Fig. 4.18), starting from the completely interconnected species (**a**), to the almost unconnected entities (**g**) is, in principle, the example of the application of percolation theory.

For the connectivity of species in each of the combinations shown in the Fig. 4.18 from **a** to **h**, it is possible to calculate Shannon entropy. Within the frame of our discussion about the possible limits in combinatorial complexity, we have to examine the correlation between the diversity (represented as entropy) and complexity. In this example, the decrease in diversity from **a** to **h** is followed by the increase in the change of entropy. As it is shown in the Fig. 4.19, the correlation of the change in entropy with the change in connectivity affords the sigmoidal curve. In accordance with our discussions, the maximum in the complexity of the inter-species connectivity appears for the structures for which the change in entropy is maximal, i.e., for graphs **e** and **f**.

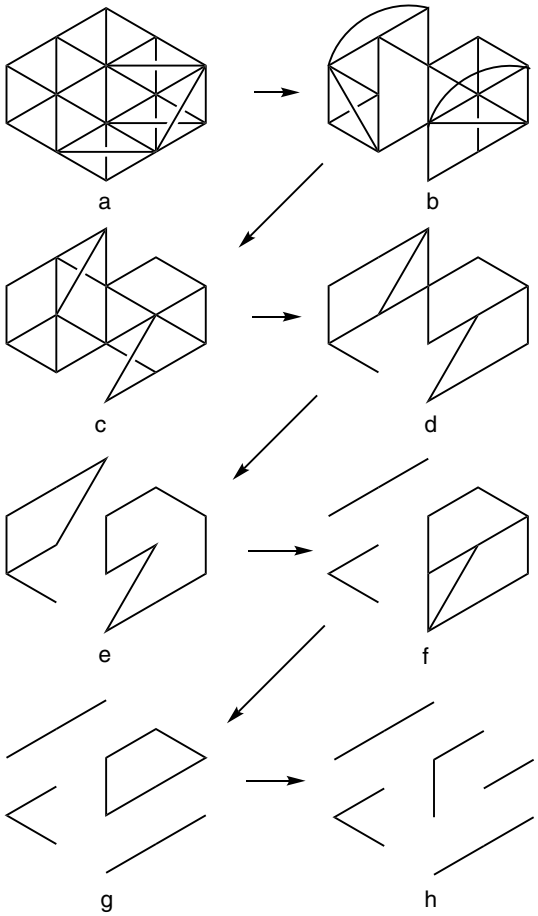


Fig. 4.18 Graph-theoretical representation of change in cohesion (connectivity) between 14 species (Adopted by permission from [36])

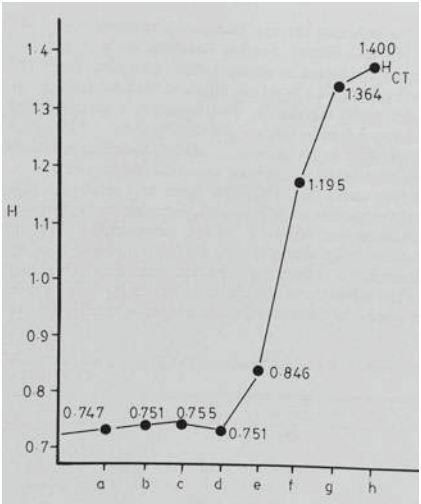


Fig. 4.19 Changes in Shannon entropy versus the changes in connectivity of the graphs representing the population of species from the Fig. 4.18 (Reproduced by permission from [36])

Thus, since the structures **e**, **f**, and **g** are positioned in the region around the inflex of the sigmoid, they are maximally complex. They represent the transition state between the homogenous diversity (**a**) and the almost empty simplicity (**h**).

4.3.2 Fractals

The discussion about the limits in combinatorial complexity requires additional representation which is based on the use of the *theory of fractals*. In short, fractals are patterns of the diminishing self-similarity. The example of the fractal structure is shown on the Fig. 4.20.

As it could easily be recognized in the Fig. 4.20, the largest figurative pattern repeats itself in continuously diminishing copies. One of the simplest examples of fractals is Koch curve (Fig. 4.21) which is named in honour to Swedish mathematician Nils Fabian Helge von Koch [37].

Self-similarity of Koch curve is based on the iterative reproduction in which the number of lines in every successive iteration is the quadruplet of the number of lines of the previous step: in the first iteration the number of lines (let us label it with N) is 4, in the second iteration the number of lines is 16, etc. The perpendicular dashed lines in Fig. 4.21 show that in every step the length of the complete pattern is diminished by dividing it with the number 3. Let us label this diminishing factor with L, thus $L = 3$. The relationship between N and L is a measure of the increase in the "density" of the fractal after each iteration. Such density is quantified with the parameter called *fractal dimension D*. The relationship between the parameters N, L, and D is described by the equation (z):

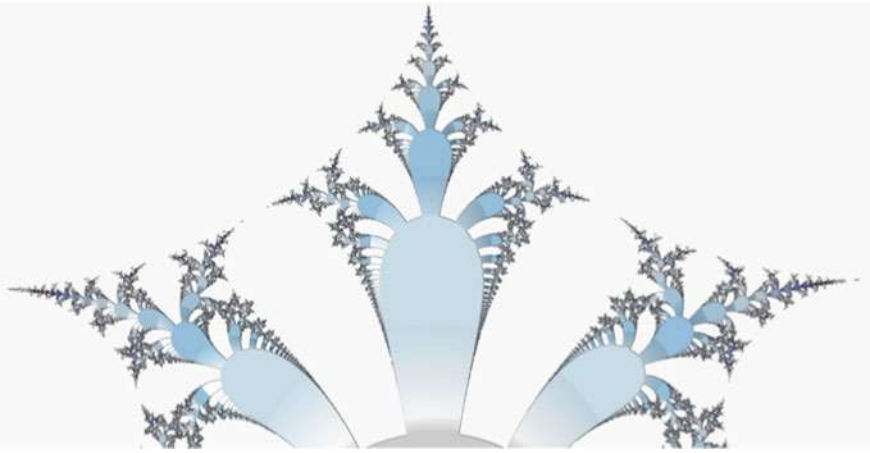


Fig. 4.20 Fractals, the structure with the diminishing reproduction of the pattern (Constructed by using the Android application Mandel Browser)

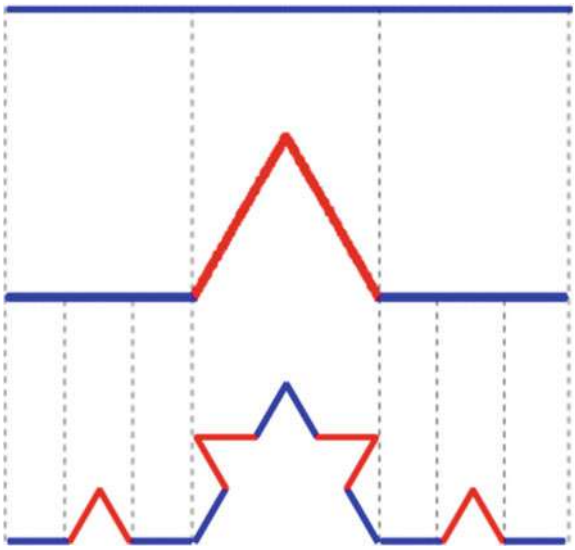


Fig. 4.21 Self-similarity of Koch curve

$$N = L^D \qquad \text{(z)}$$

The logarithmic form of the equation (z) is

$$\log N = D \log L$$

thus,

$$\log N/\log L = D$$

Fractal dimension D appears in the interval between 1 and 2, because this fractal is two-dimensional, and the maximal density of the pattern is the completely covered surface. Fractals that appear during the formation of the three-dimensional structures, as, for example, during the step-growth polymerization in the crystal phase, have the dimension between 2 and 3 [34]. Such approach is today very important, for instance, in the studies of porosity in the science of materials.

For the Koch curve represented in Fig. 4.21, the fractal dimension is 1.26186, because

$$\log(4)/\log(3) = 1.26186$$

Koch curve obtained after the millions of iterations is shown in Fig. 4.22.

Fractals can be simulated in many different ways starting with various rules for the self-repetition of patterns. Another example is the Sierpinski triangle that is shown in the Figs. 4.23, and 4.24 [38].

As it is shown in the Fig. 4.24., in the first iteration, the number of the smaller triangles (black) is 3, thus $N = 3$. In every successive iteration, the edge of the triangle is half of the length of the edge of the triangle in the previous iteration (in the iteration 1, the length of the edge is two times smaller than in the iteration 0, etc.). Thus $L = 2$. Accordingly, fractal dimension for the Sierpinski triangle is

$$D = \log(3)/\log(2) = 1.58496$$

Since fractal dimension is one of the characteristics of combinatorial complexity, it is important to examine how it is correlated with diversity. Since the diversity can be characterized by Shannon entropy, this correlation is reduced to the relationship between the Shannon entropy and fractal dimension. Fractal growth depends on the starting rules by which the n-th iteration is formed by diminishing repetition of the pattern in (n-1)-st iteration. The example of the fractal systems iteratively developed by starting with the nine different rules of grow is represented in the Fig. 4.25 [39].

Fractal dimensions for all these fractal combinatorial systems (from ***a*** to ***i***) are listed in the Table 4.2. These fractals differ in their combinatorial complexity. While the fractal ***a*** (on the top of the Fig. 4.25) represents the simplicity, the fractal ***i*** (on the bottom) is at the limit of the chaotic continuum that have a statistically compact description. Maximum complexity affords the fractal system ***f***, which is in the middle. Interestingly, the fractal dimension of the system ***f*** is equal 1.631, i.e., it is very close to the fractal dimension of the Sierpinski triangle (1.58496). It seems that the maximal combinatorial complexity appears for the structures which have fractal dimension close to 1.6.

The data in the Table 4.2 demonstrate also, that the values of the information (i.e., Shannon) entropy almost correspond the values of fractal dimensions. Maximal complexity is found for the fractal systems e, and f with the values of the entropies 1.609, and 1.792, respectively. These numbers are close to the value of *Golden ratio*

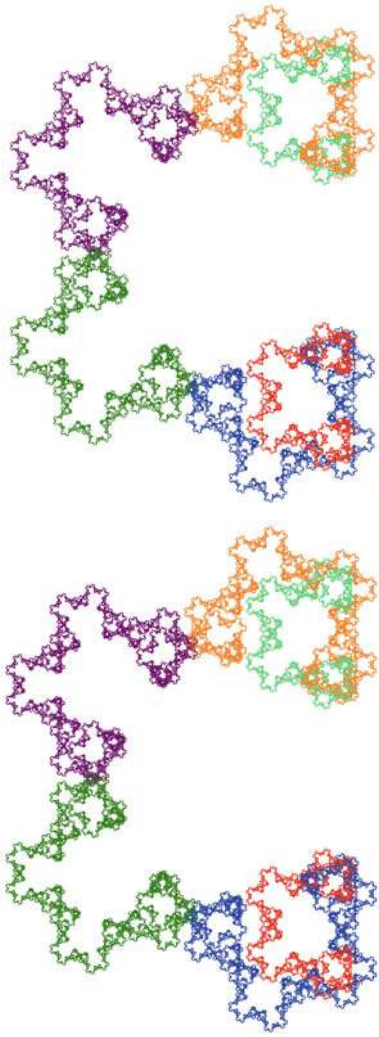


Fig. 4.22 Koch (5,0.4) curve obtained after 7 iterations (upper picture), and after one million of iterations (lower picture) (Tamás, 2010) (Courtesy of Professor emeritus Larry Riddle, Agnes Scott College, Decatur, GA)

which is nearly 1.618. During the fractal analysis of the texture of the biological species *goose down*, Gao [40] has calculated, and experimentally confirmed that the morphological texture of this species is a sort of fractal with the fractal dimension of 1.66. In the simulation studies of the fractal-type biological evolution, Zander has calculated the similar values of the Shannon entropies (1.59, and 1,43) [41]. In other studies about the self-similarity in biological developments represented as the tree-like growth, the fractal dimensions were 1.62 [42, 43]. These numbers are also very close to the Golden ratio. In the studies about the fractal nature of the branching of neurons, the fractal dimension falls between 1.4 [44] and 1.8 [45]. In this research the authors have argued that the D value varies depending on the importance of

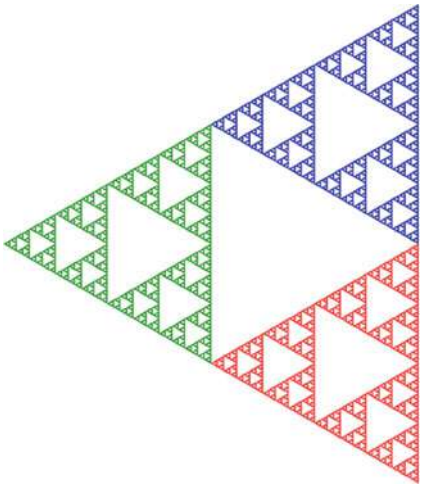


Fig. 4.23 Sierpinski triangle (Courtesy of Professor emeritus Larry Riddle, Agnes Scott College, Decatur, GA)

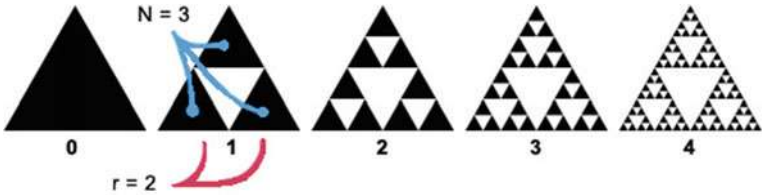


Fig. 4.24 Fractal dimension of the Sierpinski triangle (from the public website https://fractalfoundation.org/OFC/OFC-10-3.html)

Table 4.2 Fractal dimensions and Shannon-type entropies for nine growing fractals (a–i) represented in the Fig. 4.3.2.6 (Reproduced by permission from [39])

Figure	Fractal dimension	Shannon entropy	Remark
a	0.000	0.000	A point (non-fractal)
b	0.631	0.693	Cantor set
c	1.000	1.099	A straight line
d	1.262	1.386	Fractal dust
e	1.465	1.609	Box fractal
f	1.631	1.792	Complexity maximum
g	1.771	1.946	
h	1.893	2.079	Sierpinski carpet
i	2.000	2.197	A square (non-fractal)

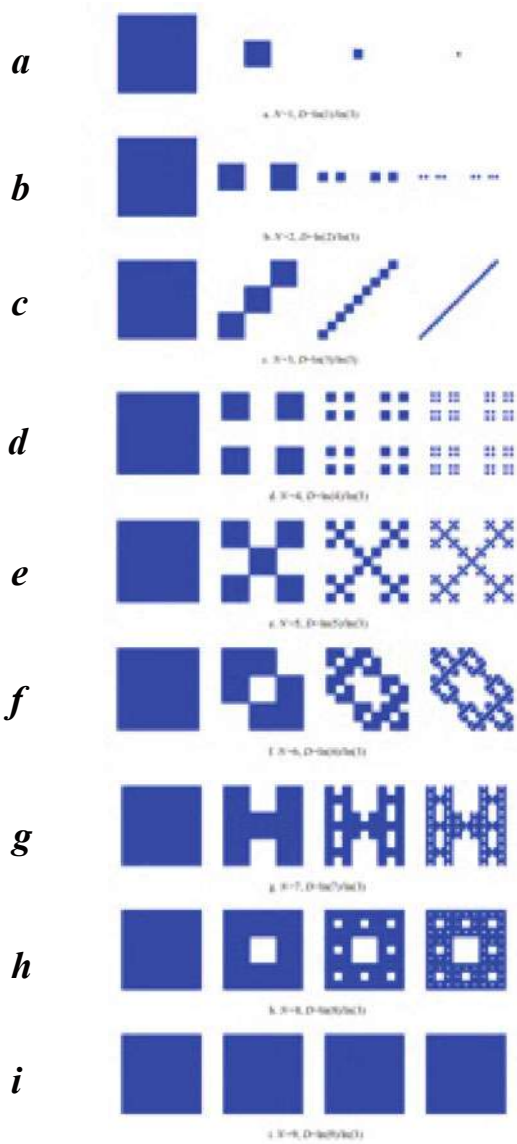


Fig. 4.25 Different fractal iterations, from top down (from ***a*** to ***i***), which form fractals of different combinatorial complexity (Reproduced by permission from [39])

the interneuron connectivity. Since the morphology of a lot of organisms follow fractal growth, what is recognized by the appearance of the Fibonacci sequence, it is possible that the biological **evolution converges to the maximum of complexity, i.e., the complexity in which the fractal dimension as well as the information entropy approach to the Golden ratio.** Interestingly, the Golden ratio (ϕ) is in simple mathematical relation also with the first Feigenbaum constant δ (which has been defined on the beginning of this book) [46]:

$$\delta \cong 2\phi/\log 2$$

Convergence in the biological evolution to the predictive morphological types of high complexity is already well studied [47–49]. I argue here, that these morphological convergent structures appear within the zone of the maximum of the combinatorial complexity.

4.3.3 One-Dimensional Fractal Dimension?

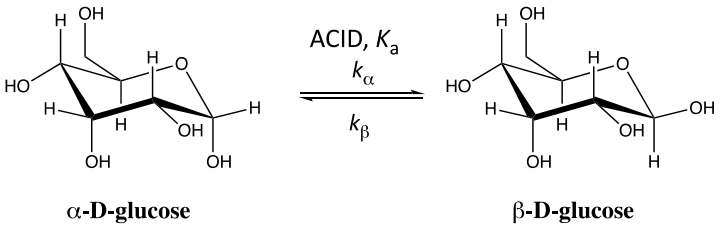
Since it is known that the fractal dimension of the two-dimensional fractal can maximally be 2, and the fractal dimension of the three-dimensional fractal can reach 3, the fractal dimension of the one-dimensional fractal, if it exists at all, should have the maximal value 1. But, what is the example of the one-dimensional fractal dimension, or, at least, is there an one-dimensional analogy to the concept of fractal dimension? The analogy we can find in chemistry, particularly, in some of the approaches in physical-organic chemistry. Almost hundred years ago Johannes Nicolaus Brønsted, and Thomas Martin Lowry [50, 51] have discovered that the rates of some chemical reactions depend on the acidity of medium. Such a *law of general acid catalysis* serves to predict the sensitivity of the rates of chemical reactions on the strengths of the acids which is extra added to the reaction mixture. For instance, the conversion of α-D-glucose to β-D-glucose (Scheme 4.1) is catalysed with acid whose strength is characterized by the value of the so called acidity constant K_a.

The rate of chemical reaction, particularly for the glucose transformation in the Scheme 4.1, is characterized with the value of the rate coefficient k_α. The dependence of this rate coefficient, k_α, on the strength of the acid catalyst, K_a, is represented with the Eq. (4.1).

$$k_\alpha = K_a^d \tag{4.1}$$

Logarithmic form of this equation is

$$\log k_a = d \log K_a + C \tag{4.2}$$



Scheme 4.1 Conversion of α-D-glucose to β-D-glucose catalysed by acid

For C = 0, we obtain the relation (4.3),

$$\log k_a = d \log K_a \tag{4.3}$$

which can be rewritten to the Eq. (4.4):

$$\log k_a / \log K_a = d \tag{4.4}$$

Equation (4.3) is the linear relationship which can be represented with the graph in the Fig. 4.26. The coefficient d is the slope of the line (tg α). It is not difficult to observe that the Eq. (4.4) is equivalent to the equation for the fractal dimension, i.e., $\log N/\log L = D$. Accordingly, the sensitivity of the rate of the acid-catalysed reactions (d) on the strength of the added acid could be recognized as a sort of the one-dimensional fractal dimension.

In this case, the value of the one-dimensional fractal dimension is within the interval between 0 and 1. If $d = 1$, the reaction is strongly dependent on the strength of the added acid, but if d is close to zero, the reaction is not catalysed by acid at all.

However, this example which has been borrowed from chemistry requires deeper explanation. In theory, every chemical transformation of one substance to another is called chemical reaction. This process can be described by chemical equations in which the formulas on the left side represent the substances before the transformation, the *reactants*. The chemical formulas of the substances that appear after

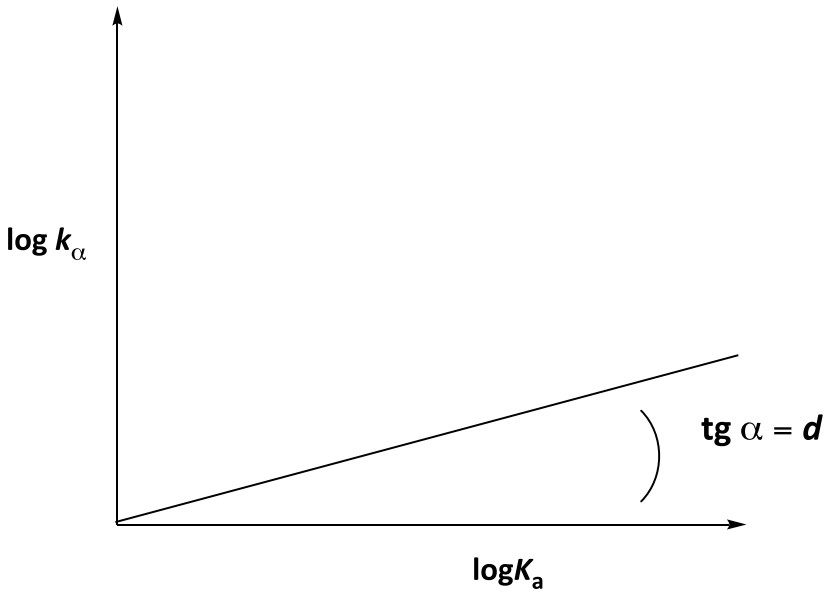


Fig. 4.26 Linear dependence of the logarithm of the reaction rate on the logarithm of the acidity constant in acid catalysed reaction

the chemical process, the *products*, are shown on the right side of the equation. For instance, if hydrogen and oxygen produce water, hydrogen and oxygen are reactants, and water is the product. In the example described in the equation (a), the chemical reaction is the transformation in which the positive hydrogen atom, the proton (H^+), is transferred from the substance characterized with the formula ROH to the substance characterized with the formula R'OH. Thus, the protonated form of ROH, the $ROHH^+$, donates proton, H^+, to the substance R'OH. Consequently, the products of this reaction are ROH and $R'OHH^+$. The proton that is transferred in this reaction is in the previous phrase labelled in red. In summary the reaction is represented with the following equation:

$$\mathrm{ROH_2^+} + \mathrm{R'OH} \xrightarrow{\text{ACID}} \mathrm{ROH} + \mathrm{R'OH_2^+} \tag{a}$$

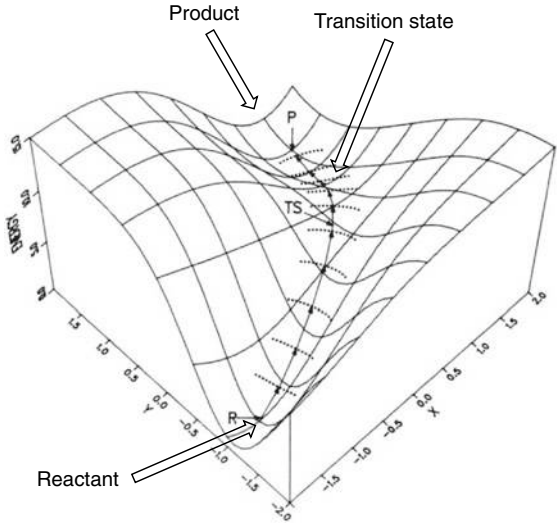
The chemical reaction which is described by the Eq. a can progress only if some *acid* is added to the reaction mixture. Thus, this reaction is acid-catalysed.

Now, let me explain the question about the nature of chemical reaction in some more details. Every non-spontaneous transformation in the physical world requires some energy which is necessary for triggering this process. For instance, to demolish the old building in the city, we first need to use a strong force that will shift the construction from its stable equilibrium. Let us call this force the *activation energy*. The same is in chemical transformations, to trigger the chemical process, i.e., to break an old or to form new chemical bond, we have to deliver some amount of the activation energy (which could be in various forms, for instance, it could be heat or radiation) to the mixture of the reactants. When the reactants absorb the activation energy, they are transformed to the state that is neither the reactant, nor the product. This state is called the *transition state*. The general concept of the transition state was already discussed in previous sections. In our example, the formation of the transition state is described by the Eq. (b).

$$\mathrm{ROH_2^+} + \mathrm{R'OH} \xrightarrow{\text{ACID}} \begin{matrix}\text{TRANSITION}\\ \text{STATE}\end{matrix} \rightarrow \mathrm{ROH} + \mathrm{R'OH_2^+} \tag{b}$$

What is the physical nature of transition states? The main characteristics of such an elusive entity is that the transition states are on the point of the highest potential energy on the *way from the reactants* (R) *to the products* (P), as it is shown in the Scheme 4.2. More precisely, the transition state (TS, in the following Scheme) appears on the "saddle point" on the potential energy surface.

The lifetime of the transition state is extremely short, it takes only about 10^{-13}-th part of the second. It is the time in which only one molecular vibration could occur. Transition states are not the commonly observable substances which are possible to keep in bottles, but rather the temporal change of the structure on the way to the final stabile form. They can be observed only by using special experimental techniques which are known as femtosecond spectroscopies. Accordingly, chemistry is not only



Scheme 4.2 Potential energy surface for the simple chemical reaction. Reproduced by permission from HB Schlegel (2023), J. Comput. Chem. 24(12), 1514-1527, DOI:(10.1002/jcc.10231)

the science about the real substances, observable by senses, but also the science about the "elusive" dynamical states. *These states have the structures of the highest complexity*.

This fact is very important for the development of the theory of complexity, because we have to discuss the structural complexity not only of the stable structures. The investigations about complexity should be extended to the complexity of the transition states. For the reaction described in Eqs. (a) and (b), the possible structures of the transition state (TS) for different values of the "fractal dimension" *d* are shown in the Scheme 4.3.

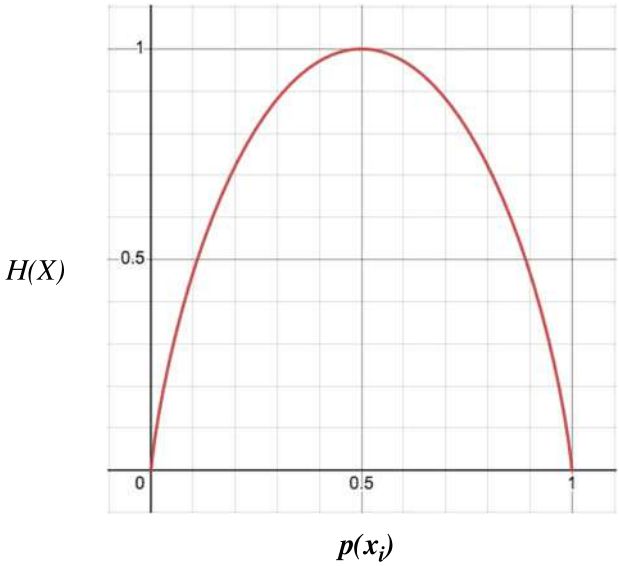
Three represented structures in Scheme 4.3. differ in the position of the proton, H^+, which is transferred from ROH to R'OH. If this reaction is not catalysed with acid, i.e., its rate is not sensitive on the presence of acid, then the transition state is *reactant-like* (i.e., its structure is similar to the structure of the reactant) because the proton is only negligibly shifted from the reactant ROH_2^+. In this case the parameter *d*, for which we have mentioned that is analogous to the fractal dimension, is almost equal to zero. On

$$ROH \dashrightarrow H^+ \dashrightarrow ROH' \qquad d \text{ is close to } 0$$

$$ROH \dashrightarrow H^+ \dashrightarrow ROH' \qquad d \text{ is close to } 1$$

$$ROH \dashrightarrow H^+ \dashrightarrow ROH' \qquad d = 0.5 \quad \text{MAXIMUM OF COMPLEXITY}$$

Scheme 4.3 The structures of the possible transition states which could appear in the reactions described with the Eqs. (a) and (b)



Scheme 4.4 Correlation between Shannon entropy and the change in the structure from the reactant to the product

the other side, if the reaction is strongly acid-catalysed, the transition state is similar to the product, R'OH_2^+, i.e., it is *product-like*. In this case the fractal dimension, *d*, is close to 1. Finally, the transition state could be more or less symmetrical with the proton H^+ between the reactant and the product molecule. In such case, *d* is close to 0.5.

Now, let us investigate the relationship between the complexities and Shannon entropy of the structure of reactant, transition state, and the product in this proton transfer reaction. By using the formula for Shannon entropy,

$$H(X) = -\sum_{i=1}^{n} p(x_i)\log_2 p(x_i)$$

$$\text{for } i = x, 1 - x$$

we can calculate the entropy for all the continuous change of all the structures from Scheme 4.3. in which the complexity is represented as the probability of the configuration on the way from the reactants to the products, $p(x_i)$, in the interval from 0 to 1. This relationship is represented in the Scheme 4.4. The maximal Shannon entropy appears for $p(x_i) = 0.5$ that corresponds to the fractal dimension $d = 0.5$ in which the transition state is symmetrical with the H^+ ion equally distant of the reactant and of the product molecule. It should be observed that, in contrast to the two-dimensional examples in the previous chapters, in this case the maximum of the entropy ($H(X) =$

1) corresponds to the maximum of the complexity (the transition state at $p(x_i) = 0.5$). This could be explained with the fact that the reactants ($p(x_i) = 0$), and the products ($p(x_i) = 1$) have the same complexity, Thus, in this example the complexity starts with simplicity (reactant), reaches the maximum of complexity in the transition state at $p(x_i) = 0.5$, and returns to the simplicity (product). In contrast, in the fractal-like two-dimensional examples, the change in complexity is not symmetrical because it begins with the simplicity, and ends in chaos.

In conclusion, such examples borrowed from chemistry represent the case of the one-dimensional fractal development in which the "fractal dimension" at the maximum of the complexity is close to 0.5. In comparison, fractal dimension at the maximum of complexity in the two-dimensional fractals approaches to 1.6, i.e., to the Golden ratio. Tentatively, is the "one-dimensional Golden ratio" close to 0.5?

4.3.4 Cellular Automata, Complexity and Shannon Entropy

The more explicit relationship between entropy and complexity we could find in the Wolfram's theory of cellular automata [52, 53]. The iterative evolution of cellular automata is determined by particular initial conditions. Starting with corresponding rules (Fig. 4.27), and with the initial conditions described as a row consisting of the combination of the black and white cells, the pattern grows stepwise, on the iterative way, to form the picture of particular complexity. The first version of such a system of cellular automata is known as the "game of life", the mathematical game invented by John Horton Conway [54]. Wolfram's patterns are constructed by using specific rules by which the figure iteratively grows starting with the first cell. For instance, *rule 30* (Fig. 4.28) requires that the cell in the succeeding row is white only in the case when three previous cells have one of the white-black combinations defined by the rule. Other rules have various combinations, which would iteratively grow to form various patterns. Wolfram has defined 256 such rules (Fig. 4.29).

By analysing the patterns obtained from all 256 rules, starting from *rule 1* to *rule 256*, it is possible to recognize the increase in complexity from maximal simplicity (*rule 1*), through the complex figures (in the middle) to the chaotic pattern represented by homogenous black surface (*rule* 256 in Fig. 4.29).

Some of the complex arrays are represented in the Fig. 4.30. It is interesting to observe that in these figures appear the patterns in which the structure is repeating itself in diminished versions, thus, they form a sort of fractals.

As I have already mentioned, depending on the rule, the different patterns appear on the scale of complexity between the simple and disordered (homogenous) limits. By calculating Shannon entropy for each of the patterns which afford different degree of complexity, it is possible to analyse the relationship between entropy and complexity. Wolfram has demonstrated that such the relationship between the entropy

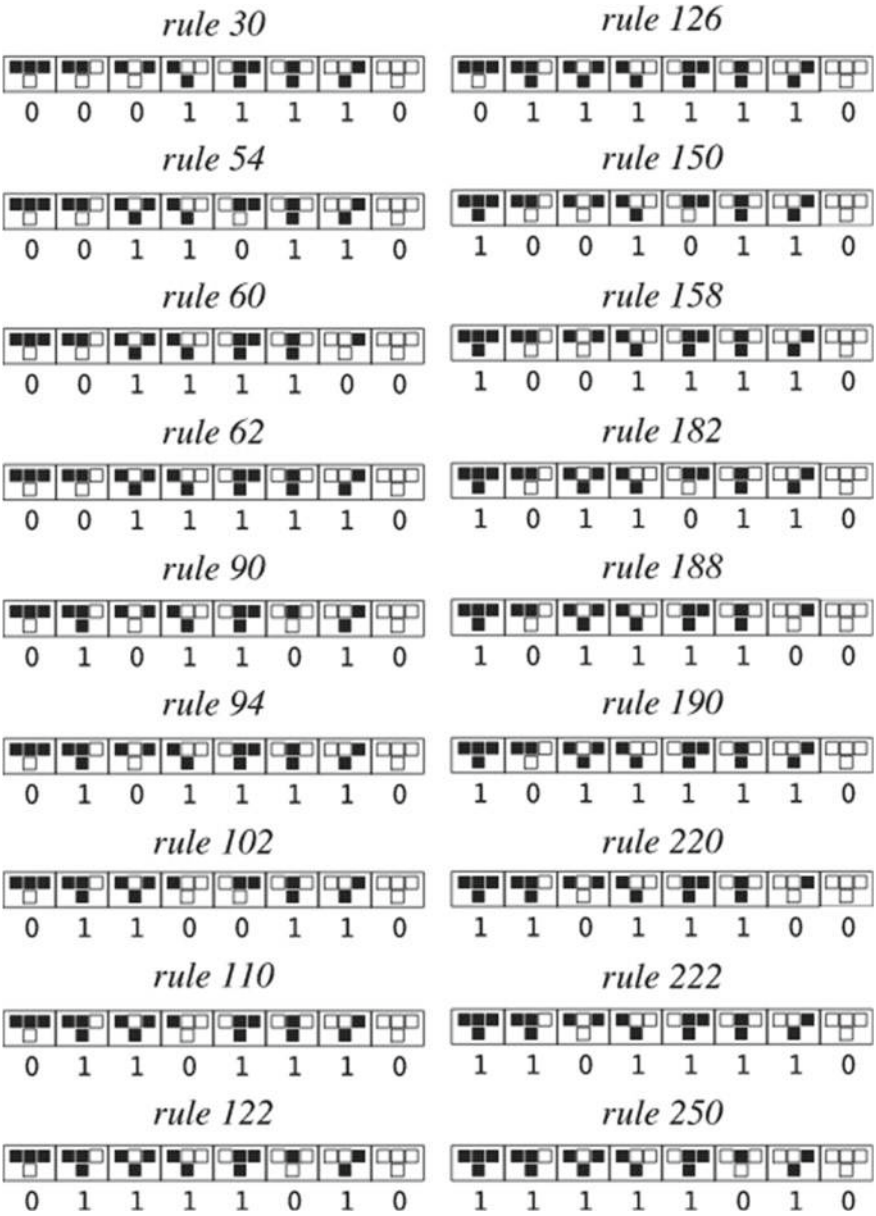
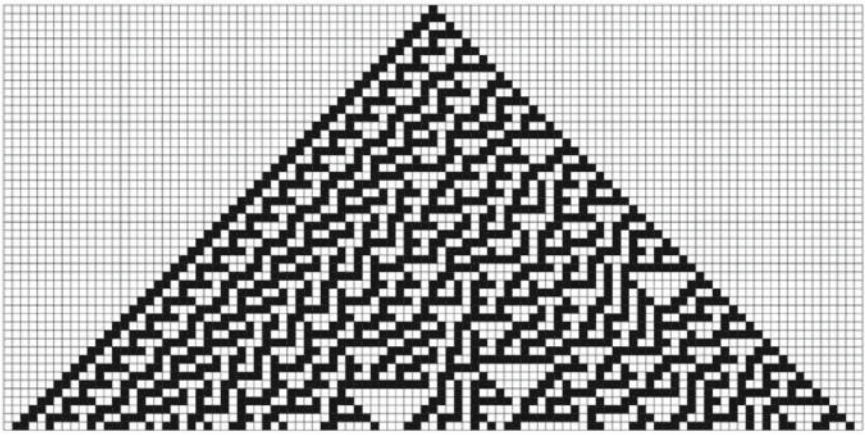


Fig. 4.27 Selection of rules for Wolfram's cellular automata (Reproduced by permission https://www.wolframscience.com)



rule 30

Fig. 4.28 The pattern using the *rule 30* of Wolfram's cellular automata (Reproduced by permission https://www.wolframscience.com)

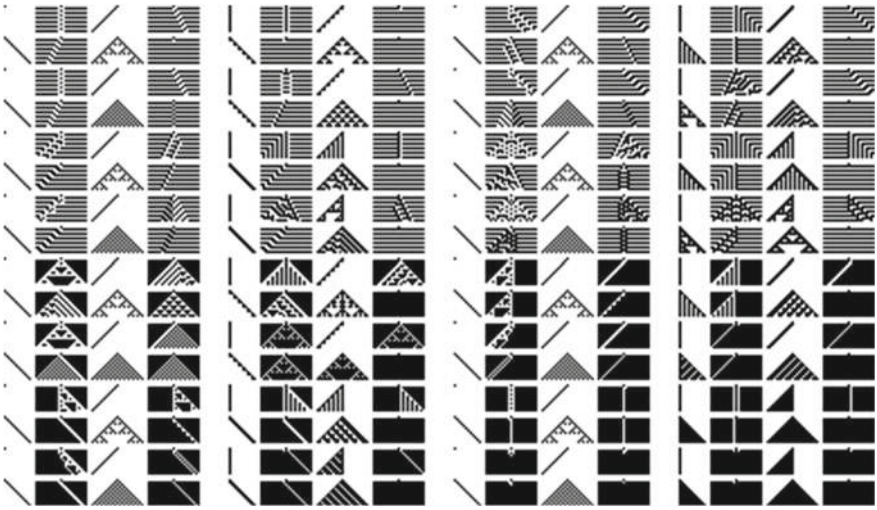


Fig. 4.29 Representation of all the 256 rules for the construction of patterns from cellular automata (Reproduced by permission https://www.wolframscience.com)

(Shannon's) and the complexity of patterns affords sigmoid curvature (Fig. 4.31). It is important to notice that one of the most complex patterns (constructed by using the *rule 109*) appear at the inflex-point of this sigmoid. Thus, the maximal complexity is limited in the zone of the largest change in entropy, i.e., on this inflex-point of the Wolfram sigmoid. This fact could be at the heart of our new intuitive *definition of the*

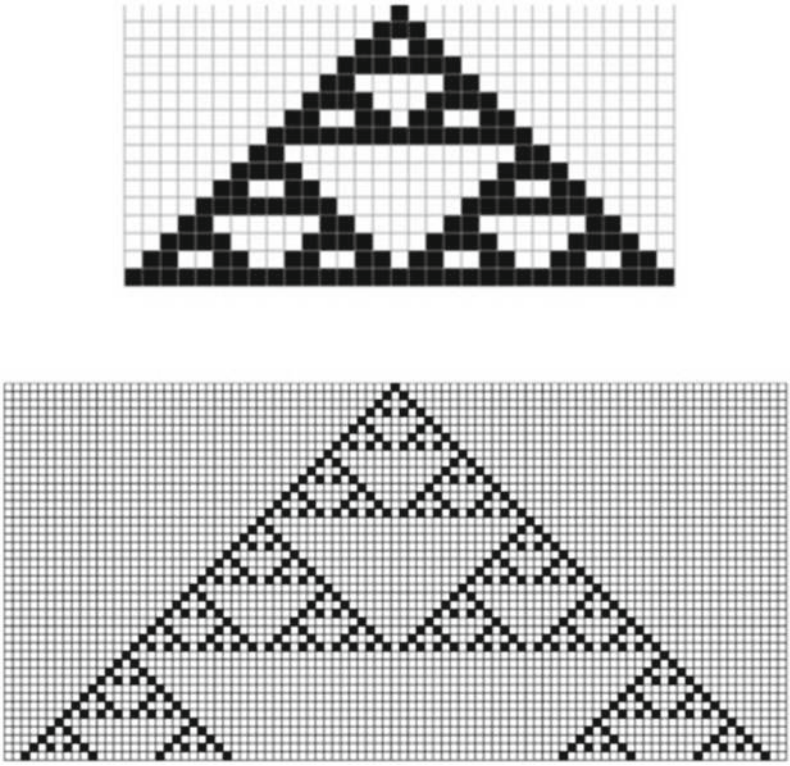


Fig. 4.30 Complex patterns formed by using particular rules (Reproduced by permission https://www.wolframscience.com)

limits of combinatorial complexity as *the state of the organization whose minimal variation causes maximal change in entropy*. In such a way, the maximal complexity is the "phase transition" between order and disorder.

As we have discussed in previous chapters, measuring of complexity involves different approaches. One of the most popular approaches is the already discussed method of Kolmogorov in which the complexity of an object is related to the complexity of its description. In the studies of the oscillatory models which are expanded between the point of the simplicity of the regular oscillations and the point of the chaotic homogeneity, complexity appears in the middle. Starting from the simple regular oscillations, the complexity grows by introducing more and more fluctuations. In the computer simulation of this transition from the simplicity to the complexity it is possible to measure the average mathematical work required to

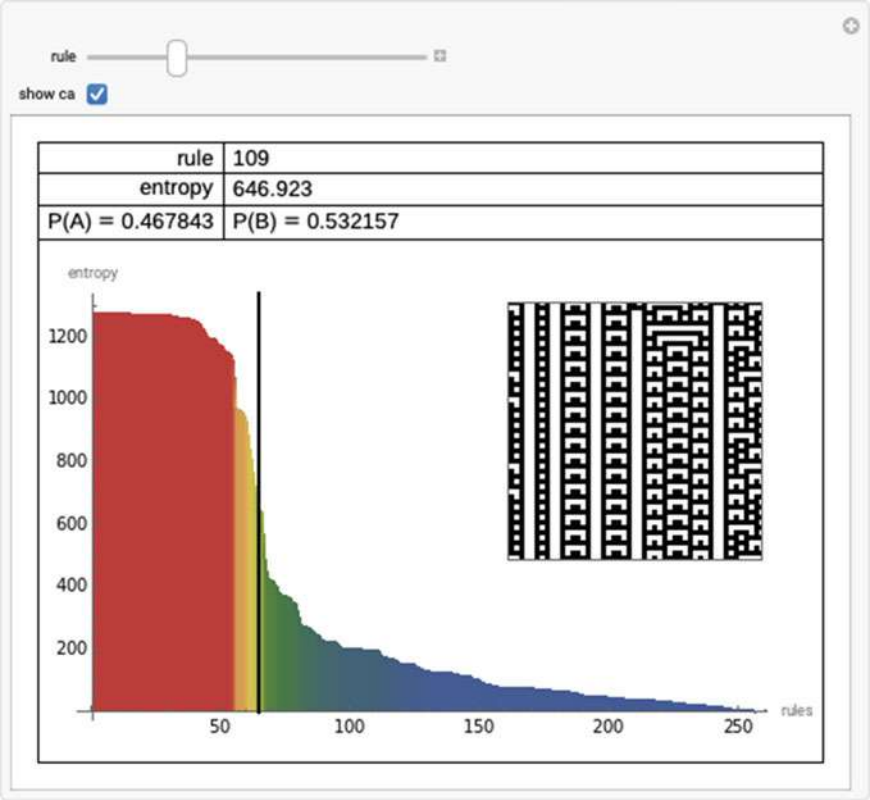


Fig. 4.31 Correlation between the lineage of Wolfram patterns of complexity and the Shannon-like entropy. The vertical line at the inflex of this diagram is the inflex point (for the pattern formed from *rule 109*) showing the maximal change in entropy (Reproduced by permission https://www.wolfram.com/legal/terms/wolfram-demonstrations-project.html)

produce a fluctuation. By studying such model by means of the graph theory, Crutchfield and Young have calculated the relationship between the calculated complexity and entropy of the graph models [55]. This correlation is represented in the Fig. 4.32.

From the Fig. 4.32 it becomes evident that the maximum in complexity dose not correspond to the maximum of the diversity expressed as the entropy. Again, we have to argue that the maximal complexity appears between simplicity and chaos. Since the peak in the Figure is sharp, the maximal complexity is characterized with the configuration whose change would cause the most prominent change in entropy.

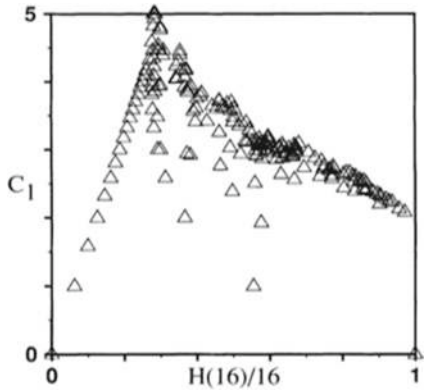


Fig. 4.32 Correlation between the complexity of the differently disturbed graph models (C_1) and entropy (H) (Reproduced by permission from [55])

References

1. Sommerer Ch, Mignonneau L (2003) Modeling complexity for interactive art works on the Internet. in "Art and Complexity" (J. Casti and A. Karlqvist, editors), Elseiver Science B.V
2. Baianu IC (2007) Categorical ontology of levels and emergent complexity: an introduction. Axiomates 17:209–222
3. Kim J (1998) Mind in a physical world. MIT Press, Cambridge
4. Simon HA (1999) The sciences of the Artificial, pp. 128, The MIT Press, Cambridge, Massachusetts
5. Vančik H (1999) Opus magnum: an outline for the philosophy of chemistry. Found Chem 1:241
6. Vančik H (2003) Philosophy of chemistry and limits of complexity. Found Chem 5:237–247
7. Vančik H (2021) Philosophy of chemistry. Springer Nature, Dordrecht, New York, Berlin
8. Poincaré H (1892) Les Méthodes Nouvelles de la Méchanique Céleste. Gauthier, Paris
9. Poschel J (2001) A lecture on the classical KAM theorem. Symp Pure Math 69:707–703
10. Plath PJ (1997) Jenseits des Moleküls. Vieweg & Sohn, Braunschweig
11. Lotka AJ (1925) Elements of mathematical biology. Dover, New York
12. Volterra V (1931) Leçons sur la théorie mathématique de la lutte pour la vie. Paris
13. Mele C, Pels J, Polese F (2010) A brief review of systems theories and their managerial applications. Serv Sci 2:126–135
14. Epstein IR (2014) Coupled chemical oscillators and emergent system properties. Chem Commun 50:10758
15. Wacquier B, Combettes L, Van Nhieu GT, Dupont G (2015) Interplay between intracellular $Ca2^+$ oscillations and Ca2+-stimulated mitochondrial metabolism. Nat Sci Rep 6:19316. https://doi.org/10.1038/srep19316
16. Saavedra M, Pérez-Mercader J, Muñuzuri AP (2022) Intermittent regimes as a synchronization phenomenon in two sets of nonlinear chemical oscillators. Chaos 32:113125. https://doi.org/10.1063/5.0104610
17. Wolfenden R (2006) Chem Rev 106:3379–3396
18. Parrilla-Gutierrez JM, Sharma A, Tsuda S, Cooper GJT, Gerardo Aragon-Camarasa G, Donkers K, Cronin L (2020) A programmable chemical computer with memory and pattern recognition. Nature Commun 11:1442
19. Kolmogorov AN (1965) Three approaches to the quantitative definition on information. Prob Inform Trans 1:1–7
20. Kolmogorov AN (1998) On tables of random numbers Theor. Comput Sci 207:387–395
21. Trinajstić N (1992) Chemical graph theory. CRC Pres
22. Yagil G (1985) On the structural complexity of simple biosystems. J Theor Biol 112:1–23

23. Polany M (1968) Lifes irreducible structure. Science 160:1308–1312
24. Randić M, Plavšić D (2003) Characterization of molecular complexity. Int J Quantum Chem 91:20–31
25. McMullin B (2000) John von neumann and the evolutionary growth of complexity: looking backwards, Looking Forwards... Artificial Life 6(4):347–361
26. Golan A, Harte J (2022) Information theory: a foundation for complexity science. Proc Nat Acad Sci United States Am 119(33):e2119089119; https://doi.org/10.1073/pnas.2119089119
27. Shannon C, Waever W (1949) The mathematical theory of communication. University of Illinois Press, Urbana
28. Huberman BA, Hogg T (1986) Complexity and adaptation. Phys D 22:376–384
29. Kauffman S (1996) At home in the universe, Penguin Books, pp 54–58
30. Hage P (1979) Graph theory as a structural model in cultural anthropology. Annu Rev Anthropol 8:115–136
31. Chomsky N (1956) Tree models for the description of language. IRE Trans Info Th 2:113
32. Broadbent S, Hammersley J (1957) Percolation processes I. Crystals and mazes. Mathematical Proceedings of the Cambridge Philosophical Society.53(3):629–641
33. Erdős P, Rényi A (2022) On random graphs. Publicat Mathem 6(3–4):290–297
34. Schamboeck V, Iedema PD, Kryven I (2019) Dynamic networks that drive the process of irreversible step-growth polymerization. Nat Commun 9:2276
35. Bibulić P, Rončević I, Varga K, Mihalić Z, Vančik H (2016) Structure and topochemistry of azodioxide oligomers in solid state. J Mol Struct 1104:85–90
36. Brooks DR, Willey EO (1988) Evolution as entropy. The University of Chicago Press, Chicago, London
37. von Koch H (1904) Sur une courbe continue sans tangente, obtenue par une construction géométrique élémentaire. Arkiv för Matematik 1:681–704. JFM 35.0387.02
38. Sierpinski W (1915) Sur une courbe dont tout point est un point de ramification. Compt Rendus Acad Sci Paris 160:302–305
39. Chen Y (2020) Equivalent relation between normalized spatial entropy and fractl dimension. Phys A 553:124627
40. Gao J, Pan N, Yu W (2007) Golden mean and fractal dimension of goose down. Int J Nonl Sci Numer Simul 8(1):113–116
41. Zander RH (2023) Fractal evolution. Zetetic Publication, St. Luis, Complexity and Systematics
42. Lv X, Wu L, Ma B (2014) The fractal dimension of the tree of life. PeerJ PrePrints. https://doi.org/10.7287/peerj.preprints.198v
43. Hilborn RC (2000) Chaos and nonlinear dynamics, 2nd edn. Oxford University Press, U.K.
44. Smith JH, Rowland C, Harland B, Moslehi S, Montgomery RD, Schobert K, Watterson WJ, Dalrymple-Alford J, Taylor1 RP (2021) How neurons exploit fractal geometry to optimize their network connectivity 11:2332
45. Takeda T, Ishikawa A, Ohtomo K, Kobayashi Y, Matsuoka T (1992) Fractal dimension of dendritic tree of cerebellar Purkinje cell during onto- and phylogenetic development. Neurosci Res 13(1):19–31
46. Smith RD (2013) Period doubling, information entropy, and estimates of Feigenbaum's constants. Intern J Bifurc Chaos 23(11):1350190. https://doi.org/10.1142/s0218127413501903.DOI:10.1142/s0218127413501903
47. McGhee GR (2011) Limited forms most beautiful. MIT Press
48. McGhee GR (2015) Limit in the evolution of the biological form: a theoretical morphologic perspective. Inter focus 5:20150034
49. McGhee GR (2019) Convergent evolution on Earth. MIT Press, Cambridge, London
50. Brønsted JN, Pedersen KJ (1924) Zeitschrift für Phys. Chemie Stöchiometrie und Verwandtschaftslehre 108:185–235

51. Brønsted JN, Guggenheim EA (1927) Contribution to the theory of acid and basic catalysis. The mutorotation of Glucose. J Am Chem Soc 49:2554–2584
52. Wolfram S (2002) The new kind of science. Stephen Wolfram, LLC
53. Wolfram S (2022) Wolfram language documentation. Wolfram Research Inc.
54. Gardner M (1970) The fantastic combinations of John Conway's new solitaire game 'life.' Sci Am 223(4):120–123
55. Crutchfield JP, Young K (1989) Inferring statistical complexity. Phys Rev Lett 63:105–108

Chapter 5
Generalizations of the Concept of Complexity

The systems theory, as it has been formulated by von Bertalanffy, talks about the holistic integration of components. In this form, the system theory overlaps with the theory of complexity. Here I wish to argue that, by looking on the methods used in their epistemology, these two theories are on the first sight equivalent. However, the rigorous analysis which is represented in this book has provided the deeper insight. While complexity could be regarded as a property, the system is more or less complex subject. Systems are composed from particular elemental units, which are interrelated in such a way that they can perform specific function in the surroundings. These elemental units of the system are complex, and their complexity is defined by the contribution of the three components of complexity: synchronic, diachronic, and combinatorial (Fig. 5.1). From the discussion in this work, it is clear that the nature of synchronic (or, structural) complexity is essentially different from the nature of diachronic and combinatorial complexities. While the synchronic complexity has a level structure that originates from the different binding energies for the formation of entities of the higher level, the change in the diachronic and combinatorial complexities appears on the scale between the homogenous and chaotic limits. Actual entities, i.e., the basic building blocks for the formation of systems, are situated in such a "complexity space". It is important to point out that such a complexity space is not based on any universal metrics. The complexity metrics is "local", and it depends only on the nature of complex objects. Accordingly, the "coordinates" in the Fig. 5.1 are not quantitative, and they have no units.

To illustrate the proposed complexity space, let us analyse the structure shown in the Fig. 5.2. Within the frame of the *synchronic complexity*, this structure belongs to the molecular level of complexity. On the scale of the *diachronic complexity*, this molecule is in the regular, repetitive vibrational state. Since this is the stable molecule, all of its vibrational modes (the changes of bond-lengths and the changes bond angles) are repetitive, and its diachronic complexity is characterized with the regular oscillations typical for the thermodynamic equilibrium. Within the frame of *combinatorial complexity*, the structure is the typical example of the fractal.

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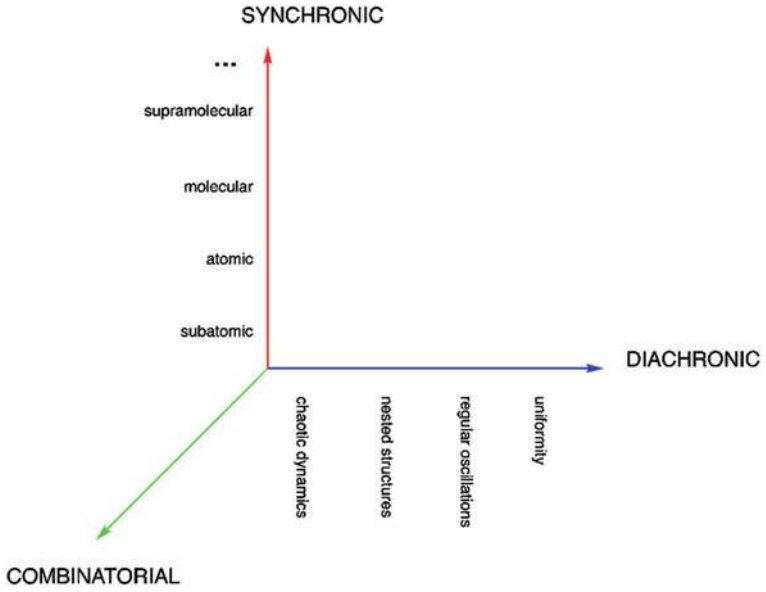

Fig. 5.1 Components of complexity, the "complexity space"

Let me now move from complexity to system. The system, as it has been defined by Bertalanffy, is composed from the elemental units of different inherent complexity. In the first sections of this work, I have called them *actualities* or *actual entities*. This term I have borrowed from the A. N. Whitehead's metaphysics in which the Universe is principally composed from the temporal units, rather than from the spatial entities [2]. Every system is formed from actualities whose complexity is characterized with synchronic, diachronic, and combinatorial contributions (Fig. 5.3). For example, different systems could consist from a variety of actualities with different positions within the "complexity space" (Fig. 5.4).

However, to form the systems, the actualities should be interconnected in the particular combinations. The interconnectivity between the actualities is a consequence of the pressure of the environment which is manifested in the requirement for accomplishing particular function. These interconnectivities between the actualities which constitute the system can be visualized by using convenient representation. In the next chapter, the systems will be represented as topological structures which can be mathematically formalized by using already discussed methods of the *graph theory*.

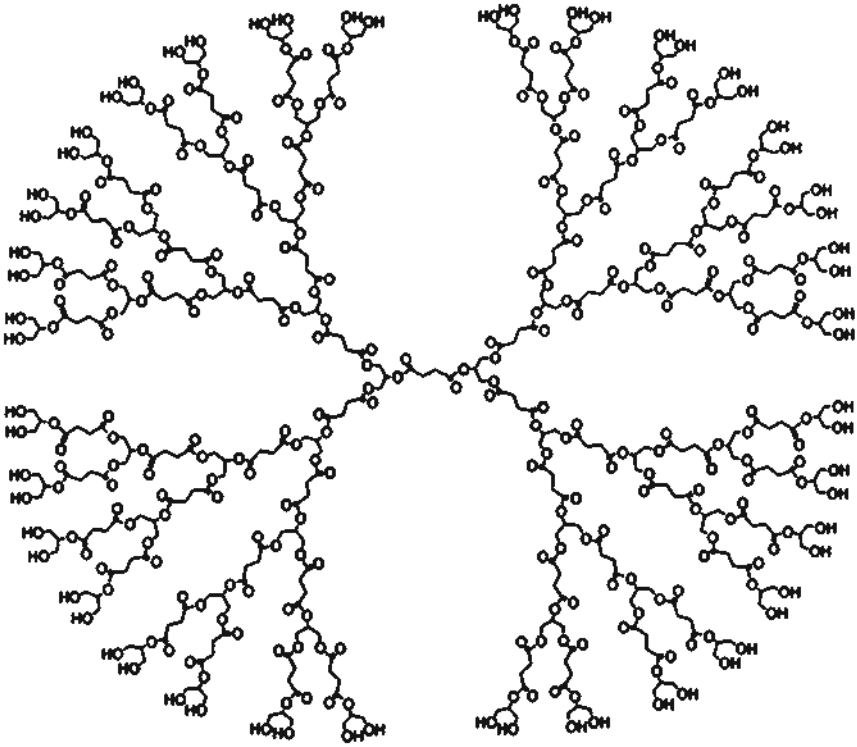

Fig. 5.2 The structure of the dendrimer molecule of poly(glycerol-succinic acid). (Reproduced by permission from Ref. [1])

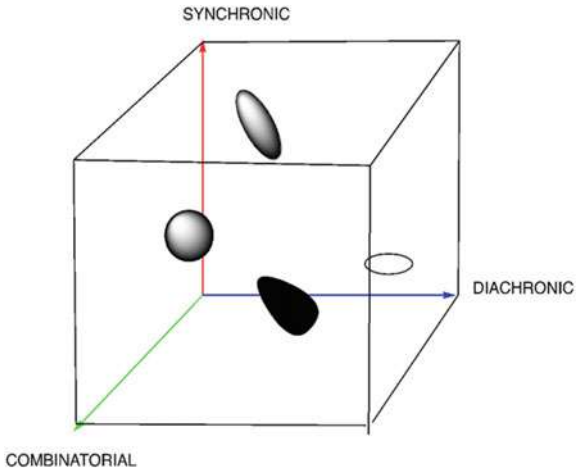

Fig. 5.3 Actualities (actual entities) as elements in constructing systems (Reproduced by permission from Ref. [3])

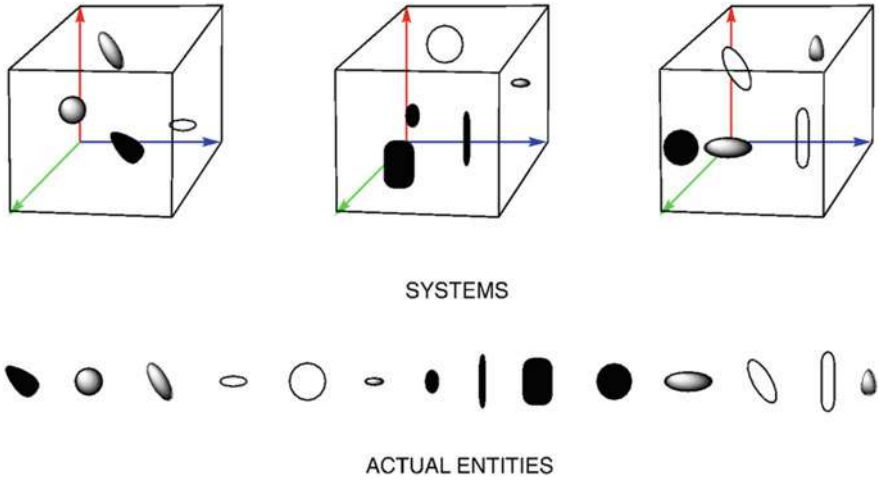

Fig. 5.4 Construction of various systems from the actualities in the "complexity space" (Reproduced by permission from Ref. [3])

References

1. Carnahan MA, Grinstaff MW (2001) Synthesis and characterization of poly (glycerol-succinic acid) dendrimers. Macromolecules 34(22):7648–7655
2. Whitehead AN (1979) Process and reality. Free Press, NY
3. Vančik H (2022) From complexity to systems. Found Chem. https://doi.org/10.1007/s10698-022-09455-6

Chapter 6
Graph-Theoretical Representation of Systems and the Problem of Function

To demonstrate the graph-theoretical representation of systems we are using two different examples in which actualities A, B, C, and D are interconnected in two combinations labelled as the system I, and the system II (Fig. 6.1). These two systems, I, and II, can be represented topologically by two different graphs (Fig. 6.1, down) [1]. As we know from the principles of the theory of graphs, such graphs could be mathematically described by matrix representations (Fig. 6.2).

The determinants of the matrices from the Fig. 6.2, which are the topological representations of the systems A, and B in Fig. 6.1, can be transformed in the polynomial of the fourth degree. For instance, the system II is represented with the *characteristic polynomial* $x^4 - 4x^2 + 2x + 1 = 0$. In graph theory, the solutions of this equation ($x_1 = -0.31$, $x_2 = -2.17$, $x_3 = 1$, $x_4 = 1.481$) are known as the *spectrum of the graph*.

It is important to be mentioned that this picture is oversimplified. The real systems should be represented with the more complex matrices whose elements can be variables, or complex numbers, etc. Depending on the nature of the interface between the system and the environment.

From the investigations of the chemical graph theory is known that, occasionally, different graphs can lead to the same spectrum (*isospectral graphs*). For instance, Hosoya has represented two graphs that are shown in Fig. 6.3 [2].

Since the graphs represented in the Fig. 6.3 are different, their adjacency (distance) matrices and the corresponding determinant **D**(A) and **D**(B) are also different (Fig. 6.4). However, the solutions of both the determinants led to the *same characteristic polynomial*:

$$x^8 - 15x^6 - 12x^5 + 41x^4 + 28x^3 - 35x^2 - 12x + 9$$

The solutions of this polynomial, x_1 to x_8, represent the graph spectrum which is the same for both the graphs A, and B.

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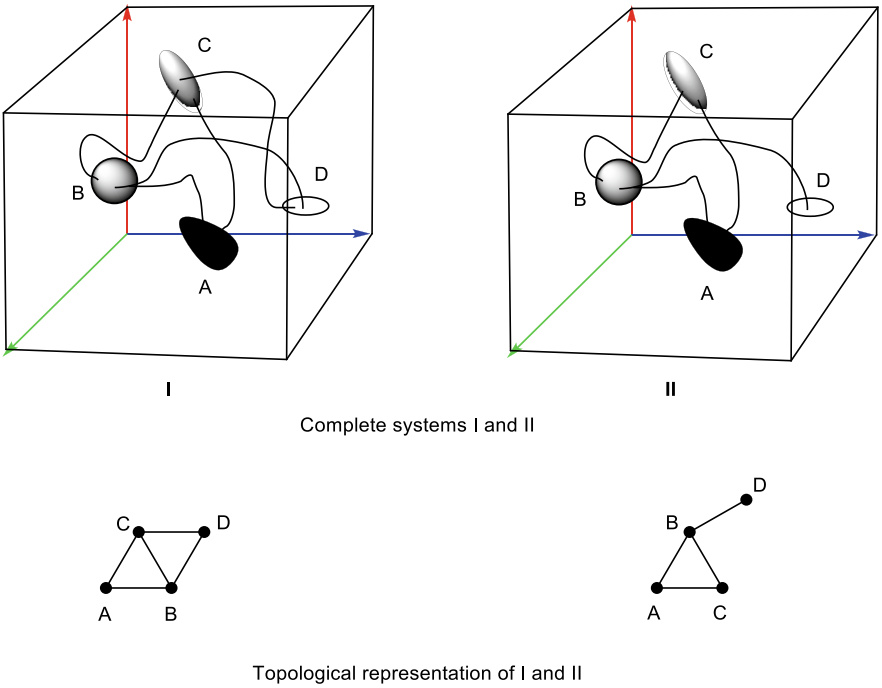

Fig. 6.1 Representation of two different systems as topological objects. (Reproduced by permission from Ref. [1])

$$\begin{bmatrix} x & 1 & 0 & 1 \\ 1 & x & 1 & 1 \\ 0 & 1 & x & 1 \\ 1 & 1 & 1 & x \end{bmatrix} \qquad \begin{bmatrix} x & 1 & 1 & 0 \\ 1 & x & 1 & 1 \\ 1 & 1 & x & 0 \\ 0 & 1 & 0 & x \end{bmatrix}$$

SYSTEM **I** SYSTEM **II**

Fig. 6.2 Matrix representation of the graphs of systems from Fig. 6.1

What we can conclude about the nature of systems from the application of such graph-theoretical representation. Systems are holistic, and the characteristics of systems is their role in expressing particular function which originates from the impact of the environment. If a **system** is modelled by a graph, its **function** is represented by corresponding **graph spectrum.** Since different graphs, as models

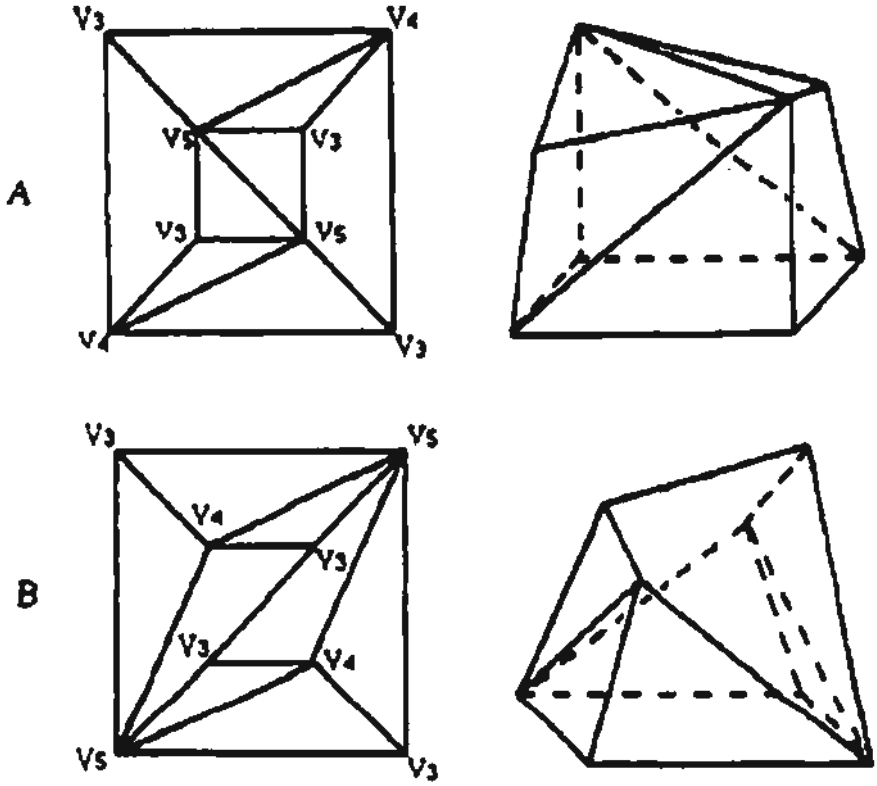

Fig. 6.3 Isospectral graphs. (Reproduced by permission from Ref. [2])

distance matrix

$$D(A) = \begin{bmatrix} 0 & 1 & 1 & 2 & 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 1 & 2 & 2 & 2 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 2 & 2 \\ 2 & 1 & 1 & 0 & 2 & 1 & 2 & 2 \\ 2 & 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 2 & 2 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 2 & 2 & 2 & 1 & 1 & 0 & 1 \\ 2 & 1 & 2 & 2 & 2 & 1 & 1 & 0 \end{bmatrix} \quad D(B) = \begin{bmatrix} 0 & 1 & 1 & 2 & 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 1 & 2 & 1 & 2 & 1 \\ 1 & 1 & 0 & 1 & 2 & 2 & 1 & 2 \\ 2 & 1 & 1 & 0 & 1 & 2 & 2 & 2 \\ 2 & 2 & 2 & 1 & 0 & 1 & 1 & 2 \\ 2 & 1 & 2 & 2 & 1 & 0 & 1 & 1 \\ 1 & 2 & 1 & 2 & 1 & 1 & 0 & 1 \\ 2 & 1 & 2 & 2 & 2 & 1 & 1 & 0 \end{bmatrix}$$

Fig. 6.4 Matrix representation of two isospectral graphs from Fig. 6.3. (Reproduced by permission from Ref. [2])

for systems, can be isospectral, as it is the case shown in Fig. 6.4, then *different systems can perform the same function, they are isofunctional*. The activity of the isofunctional enzymes is very well known from biochemistry.

This approach could also explain the principle of *supervenience*. Supervenient are the properties that appear at particular level of complexity, and which can be caused by various origins from the lower complexity level. For instance, the red colour is the supervenient property (that appear on the visual level of complexity) because it could appear as a result of the spectra of substances on the lower complexity level, characterized with quite different molecular structures. Thus, different molecules (lower level) can afford the same colour (higher level). But, oppositely is not possible, i.e., that different colours (the spectra) appear from the same microscopic configuration. In graph theory, the spectrum of the graph supervenes their causal origins, i.e., the various interconnections of the vertices in the isospectral graph. In the real world, the colour of a substance is a visual effect caused by its electronic spectrum. As we know from quantum theory of molecular spectroscopy, electronic spectrum, as well as the appearance of colour, is the consequence of the transitions of electrons between different energy levels. Already from the Hückel theory we know that the electronic structure of molecules can be deduced from their graph properties. Consequently, graphs and the spectra of graphs calculated from corresponding determinants are also correlated with the spectra of the visible and ultraviolet light. The empirical visual property of a substance composed of molecules is its colour. As we have explained, the colour is the visualization of the molecular spectrum. If different substances can have the same colour, they are in the same time also isospectral. In such a way, the colour as a *function* of the molecular system in the biological level, supervenes the molecular level of complexity. Thus, different molecular systems can exhibit the same function, the colour, and they are isofunctional in expressing the colour. In ecological systems the sensitivity to particular colours is very important function which has been in living beings developed in accordance with the specific impact of the environment, the spectrum of the Sun. The system is in such a way formed teleologically by the impact from outside.

It is very well known from the theory developed by von Bertalanffy, that one of the most important characteristics of systems is their *equifinality*: structurally different systems, or the systems developed from quite diverse starting conditions can evolute to perform the same final function. In our example, isospectrality can serve as one of the possible models for the explanation of equifinality.

The more general problem of *function* has been discussed by Polany [3] and Deacon [4]. Both the authors agree that function origins from the environment and its impact, which induces the formation of system is the introduction of the constrains on the physical laws. Such constrains enables the formation of systems which can perform some specific function. It is important to point out that the function in smaller system is shaped by the requirement of the larger system. For instance, the enzyme DNA polymerase has the function to replicate DNA. But this replication function is a part of the higher level function such as growth and the development of organism [5].

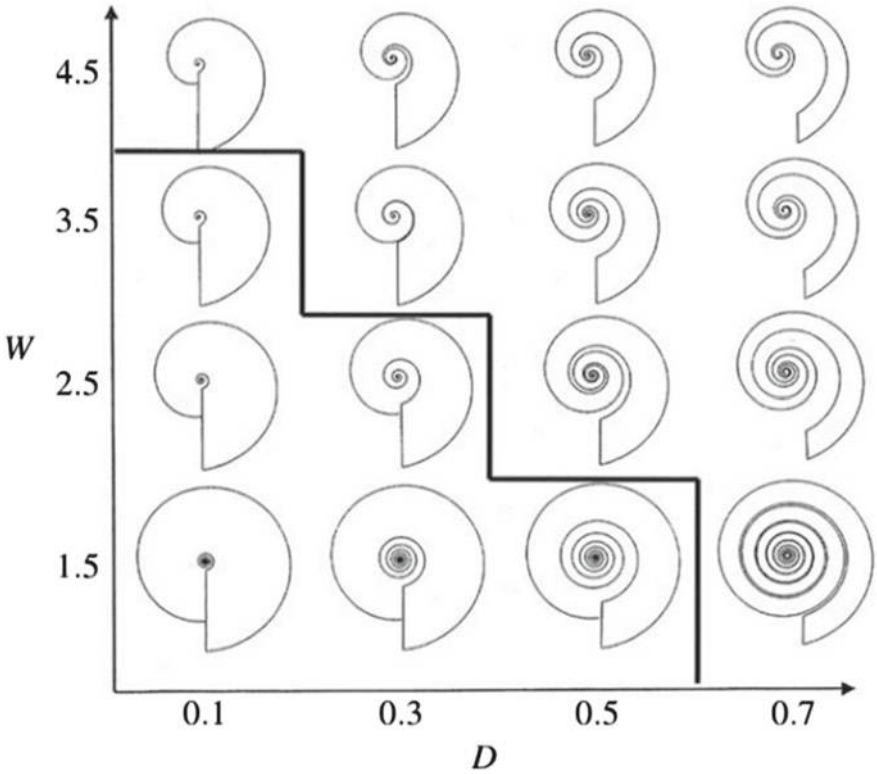

Fig. 6.5 The example of the continuous change in the morphological forms (*D*) with the rate of growth (*W*) of models of *ammonoids*. (Reproduced by permission from Ref. [2])

The deeper insight into the problem of function can be drawn from the theoretical analysis of the *morphospace* in the studies of the evolution in biology. McGhee [6] has developed the theoretical model by which it is possible to distinguish and to predict the typical morphological forms of the species that are expectable in evolution. Theoretical morphospace is the *n*-dimensional space in which the systematic changes of morphological form are correlated with the rate of the growth. The example of such an analysis is represented in the Fig. 6.5.

Of all the represented possible forms in Fig. 6.5, only those that are in the polygon boundaries shown in the lower left corner exist in the nature. This is a consequence of the pressure of the environment: only forms from the lower left corner satisfy the requirements to perform the functions which has appeared as an impact of the environment. From the general point of view, the pressure of the environment is the consequence of the structure of the Universe on the most fundamental level. McGhee has proposed the radical conclusion by which the evolution is convergent, it is constrained with the predictable set of morphological forms. Such *limitations in*

the evolution are the immediate consequence of the limits in complexity, which has been discussed in this book.

In the analogy with the morphospace analysis, similar pressure of the environment that origins from the basic laws of nature can be demonstrated on the development of constitutions of hydrocarbon molecules. By using the graph-theoretical approach, it is possible to construct enumerate number of the constitutions of possible molecules starting with particular number of vertices which represent atoms [7]. For instance, without the pressure of the environment, i.e., in this particular case without the determined valency of chemical elements, some of the possible constitutions consisting from 10 vertices are represented in Fig. 6.6. These structures were constructed without the pressure of the environment. i.e., without the limitation of the valency of each vertex.

However, the pressure of the environment, the laws of quantum mechanics, for example, can form only the structures with the limiting valency of atoms. In the case of hydrocarbons, the valency of the carbon atom is 4. Consequently, of all the possible structures only those that satisfy the valency of carbon to be 4 can exist in the nature. The list of such structures is much smaller (Fig. 6.7).

The problem of the decisive pressure of function on the development of biological systems is one of the basic questions in the theory of evolution. While McGhee argues that the evolution is limited and predictable [8] because it produces the typical forms or patterns, Kauffman claims that evolution is potentially unbounded in diversity and, consequently, unpredictable [9]. As the argument for his opinion Kauffman has used an analogous example from the practical life. Kauffman is asking whether is it possible to list all the imaginable functions of a screwdriver, which, for instance, could be used to screw, to open a can, wedge open a door, etc. Kauffman's conclusion is that the uses of screwdriver are in principle indefinite. Accordingly, there is no algorithm which could list all the functions of screwdriver. With such argumentation, Kauffman asserts that the function of an entity (for example the enzyme) is defined in evolution a posteriori. The additional Kauffman's argument is that evolution itself produces new functions that are in principle unpredictable. Hordjik [10] has proposed the compromise between two extreme statements explaining that McGhee concept is based on the final *biological forms or patterns*, but Kauffmann is focused on *functions*. In the frame of our interpretation of the systems, the screwdriver is not an accidental entity. Rather, it is a *consequence* of the evolution in technology caused by pressure of function from the environment (to drive screws). An indefinite list of its uses is not crucial for the explanation of evolution. The *screwdriver is a lever*, the *simple tool that has wide applications*, rather than specific function. Accordingly, a screwdriver is not an appropriate model for such argumentation.

In the frame of our concept about limits in complexity, McGhee's idea is more acceptable. Within our theoretical frame, (i) evolution converges to the maximum of complexity, i.e., to the state whose change would cause the largest change in entropy, and (ii) it forms the higher complexity levels until the energy of interactions between entities which should led to the higher complexity level is so small that higher forms are unstable and not sustainable (because of the synchronic complexity constrain).

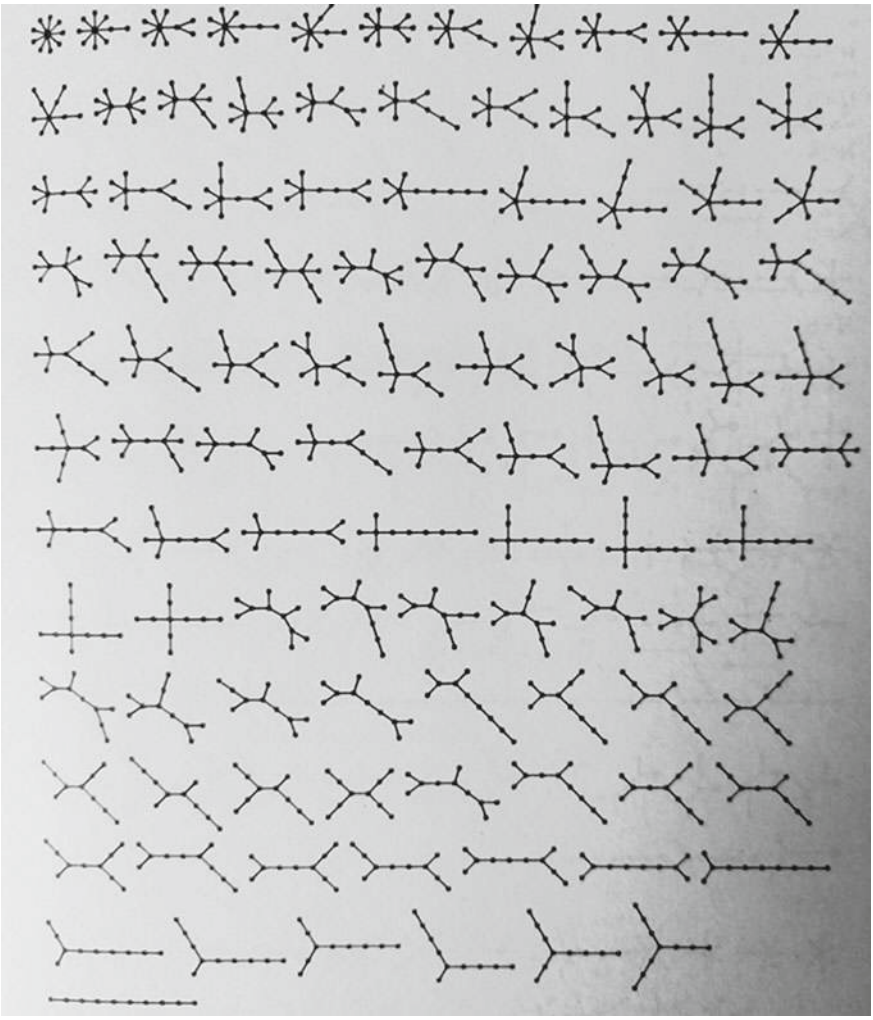

Fig. 6.6 All the possible structures represented as graphs consisting of 10 vertices in which the valency of the vertex is not limited. (By permission from Ref. [7])

The maximal complexity appears for the collections of entities (actualities) which are able to form the teleologically consistent system. For instance, the collection of 20 amino acids is the base for the formation of the *functional* protein molecules with the highest complexity. Let us imagine the protein molecule consisting from a large number of various amino acids which appear on the combinatorial complexity coordinate which is correlated with the growth of the diversity: from the simplest peptides consisting only from one type of amino acid to the chaotic continuum of the folded protein molecules consisting from hundreds of different amino acids. The

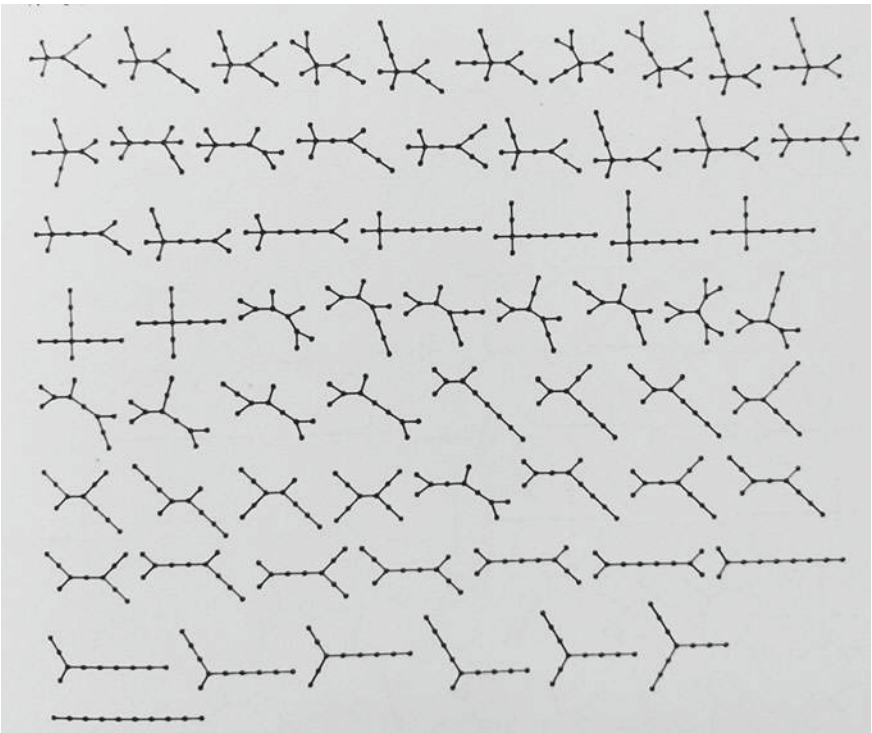

Fig. 6.7 All the possible structures represented as graphs consisting of 10 vertices in which the valency of the vertex is limited to 4. (By permission from Ref. [7])

maximum of the combinatorial complexity appears for the combination of natural 20 amino acids because only such proteins are functionally optimal.

References

1. Vančik H (2022) From complexity to systems. Found Chem. https://doi.org/10.1007/s10698-022-09455-6
2. Hosoya H, Nagashima U, Hyugai S (1994) Topological twin graphs. Smallest pair of isospectral polyhedral graphs with eight vertices. J Chem Inf Comput Sci 34:428–431
3. Polany M (1968) Lifes irreducible structure. Science 160:1308–1312
4. Deacon T (2008) Shannon–Boltzmann–Darwin. Cogn Semiot 2:167–194
5. Slater M (2009) Macromolecular pluralism. Philos Sci 76(5):851–863
6. McGhee GR (2015) Limit in the evolution of the biological form: a theoretical morphologic perspective. Interface Focus 5:20150034
7. Knop JV, Müller WR, Szymanski K, Trinajstić N (1985) Computer generation of certain classes of molecules. SKTH/Kemija u industriji, Zagreb
8. McGhee GR (2011) Limited forms most beautiful. MIT Press

9. Kauffman S (2016) Beyond Pythagoras: no laws entail evolution. Lecture presented at the Konrad Lorenz Institute, Klosterneuburg, Austria. https://www.youtube.com/watch?v=EWo7-azGHic
10. Hordijk W (2016) Evolution: limited and predictable or unbounded and lawless. Biol Theory 11:187–191

Chapter 7
Philosophical Consequences

Explorations in this book, which are focused on the relationship between the theories about the complexity and the theory of systems have in the first place the purpose to reshape at the least some of the general considerations in the philosophy of science. On the first place, this research deals with the systems as evolutive objects, independently whether they appear in biological, or in the chemical/physical evolution. As such, these evolutive entities, whether they are atoms, molecules, living beings or higher structural aggregates were formed through their particular histories. Consequently, systems, as well as other objects that are developed through specific histories, possesses their *identity* of higher order. In contrast, the identity of lower order is characteristics of the pure simple chemical substances, for instance, such as water. This identity of the substance means that wherever, or by whatever process the particular stuff has been formed it is characterized by the same lower-level identity. Water is the same substance independently whether it has been prepared from hydrogen and oxygen in the laboratory, or if it was produced in the interstellar chemical processes.

The history responsible for the formation of systems, which are characterized with their higher level identity, is manifested as an impact, i.e., the specific requirements, of the environment. The impact of the surroundings can appear in the form of the necessity for the execution of particular function. To satisfy the specific role of the function, the environment determines the manner by which the actualities have to be interconnected in the system. What is function? From the philosophical point, it should be more or less defined in a broad sense. Here, I wish to explain the concept of "function" on the simple way: function is the characteristics of the system which is exclusively oriented not to itself but outward, *in the direction to outside*. If the complexity in the nature has a level structure, then the actualities that belong to the lower level of complexity form systems by their meaningful co-organization. System formed in this way belong to the higher complexity level. This transition from the lower to the higher complexity level, i.e., from the level of actualities to the level of systems is the consequence of the pressure of the environment, and this pressure is in the form of function.

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The terms such as "structure" and "function" as well as the phrase "structure-function relationship of the molecule….." have appeared in the scientific literature which covers the investigations in the applied sciences, especially in the medicinal or pharmaceutical chemistry. These studies are focused on the investigations about the relationship between the structure of particular molecule and the biological function of this substance. Most of the scientist in these fields of research are not aware that the phrase "structure-function relationship of the molecule….." represent the mixing of two levels of complexity because while the structure of the synthesized molecule belongs to chemistry its function does not belong to the chemical level of complexity. For instance, if such a molecule is a sort of newly synthesised enzyme catalyst, then its structure belongs to the problematics of chemistry, but its function can be understandable only within the science that covers the biological level of complexity.

Analogous examples are in the social systems where the society shapes a function, and the individuals should reshape their actions accordingly with this social requirement. By its complexity the society belongs to the higher level structure which requires from the individual to perform social functions. In such a way, the civilised person is expected to be oriented towards the outside!

Function creates also all the technological systems: it is an inspiration for the creativity in the designing new useful devices. The role of the designer is to find the way how to constrain the actions of physical or chemical laws for performing particular function of the device that is delineated by environmental requirements. In such a way the function induces the creative act.

Systems created under the pressure of the environment consist from space-temporal entities that were in this book named *actualities*. To form the system, actualities should be interconnected on particular way. Such interconnection can be elegantly represented by using the principles of the graph theory where the actualities (or entities) are represented by vertices, and their interconnections by edges. This approach has an epistemological value because instead that we estimate the complexity of the structure of the system, we can simply visualize the complexity or its representation by matrices and their determinants. If the matrix which represent the system is complex because it is divided into smaller blocks, then the represented system is also complex. Actualities which form the system could possess different nature. They can be simple objects, but they can also be the simpler sub-systems. Consequently, the nature is complex because it encompasses systems formed from sub-systems which are formed from sub-sub-systems, and, "ad infinitum".

Actualities as units that form the systems have corresponding complexity. The basic difference between the notions of complexity and systems is that complexity is only the property, and the systems are entities. What is complexity? For the beginning, the answer should include a sort of a priori characterizations of the complexity through definition of corresponding categories. The partial categorization of complexity can be found in literature. for instance, by explaining the complexity levels.

More systematic approach is represented in this book by analysing three categories of complexity, synchronic, diachronic, and combinatorial. Such classification could

have an impact on some attitudes in the philosophy of science. The main contribution to the philosophy of science is in the field of possible constrains in complexity.

Limits of complexity appears as the central theme in almost all the previous chapters. The question about the limited or unlimited Universe has been, and it still continues to be in the core of the discussions in general science and philosophy. Debates about the boundaries of the universe were in the scientific history primarily focused to the space-temporal categories. It was during the establishment of modern science when the problem of limitations in the nature has been supplemented with the existence of the unchangeable physical constants such as the speed of light, or Sommerfeld's coupling constant, or a series of the thermodynamic constants, etc. Taking into account this fact, we have to be conscious that we live in the constrained world. Say, that the limitations of the Universe are of two types, the possibility of the space-temporal limit, and the ontological limit which origins from the fact that everything in the nature is the consequence of the particular basic physical and chemical constants.

However, investigation in the field of complexity studies have opened the question about the possibility of further confines in the nature: constrains in evolutionary developed pathways (*convergent evolution*), and limits in all the categories of complexity. The idea of convergent evolution is based on the fact that there are similar or analogous structures in the living nature that are not attributed to the common genetic cause. For instance, the structure of the palm tree appears between land plants as well as in the ocean. But in ocean, this palm-structured living being is not the plant but animal. Or, wings of the insects are shaped by the same morphological principles as are the wings of birds in spite to the fact that birds and insects are not in the same genetic line. Thus, "the number of evolutionary pathways available to life is not endless, but instead finite and limited" [1]. Criticism of this theory has been based mostly on the wrongly comprehended technical terms. The discussion has been focused on the difference between *convergent evolution* and *parallel evolution* [2]. In his book "Convergent evolution in Earth" McGhee argues that these two terms belong in principle to the same general idea.

The concept of limits in complexity discussed in this book theoretically supports the idea about the convergence during the development of particular morphological forms which have been driven by evolution. Especially, the fact that complexity is not correlated with the diversity (represented by entropy), but rather reach its maximum in the patterns whose changes in the structure cause the largest variation in entropy, is in line with the statement within the convergent evolution theory by which the forms (or their complexity) are more or less final and predictable. On the scale from the simplicity to the chaotic continuum, complexity appears in the middle [3]. Similar idea appears in a series of papers. Let me, for instance, mention the PhD Thesis of B. Edmonts who also argues that complexity appears between the simple structures and the high chaotic diversity [4]. In the fractal representation of the growth in the combinatorial complexity, the maximum of the complexity appears when fractal dimension, which is correlated with the Shannon entropy, approach some more or less constant values. Interestingly, the value of the two-dimensional fractal dimension of the most complex forms approach to 1.6, the number that is close to one of the most

Fig. 7.1 Limits of complexity in the fine art. (From left to right: Cimabue, P. Cézanne, G. Braque, and J. Pollock)

known limiting constants in the nature, the Golden ratio. Even more, this number is in the correlation with the first Feigenbaum constant.

Synchronic complexity is focused on the basic ontological structures, from molecules to the society. Such complexity has a level structure with levels of subatomic particles, atoms, molecules, molecular aggregates, etc. Every structural level is characterized by corresponding interaction energy required for the formation of the entities on the higher level from the entities on the subordinate level. As it has been discussed in detail in this book, in going from the simpler to more complex levels, this interaction energy becomes ever smaller. Consequently, complexity cannot grow ad infinitum because the interaction energies for the formation of the higher and higher levels becomes so negligible that the limiting higher level becomes highly unstable and, as such, it is not more persistent.

In conclusion, the temporarily observable Universe is confined by various limits that are inherent to it. In philosophy of science, this fact has induced various speculations such as the "weak anthropic principle" proposed by Brandon Carter by which the appearance of human beings is unavoidable because everything in the global evolution is determined by an assembly of physical constants [5].

This proposed "*Principle of the universal limitology*" can be witnessed also in the arts. In the history of Fine Art the development of the stiles has been directed from the realistic presentation of visual impression to the final abstraction (Fig. 7.1). Starting from the conjecture that the abstraction in painting is close to the maximum of complexity, the further development of the stiles in Fine Art could be questionable.

Similarly, in the development of the structures of music art, the most important has been the progress in the *harmony* (cords), *contrapunctus* (counterpoint), and rhythm. From the very strong rules in using the harmony solutions in the Renaissance, music has been developed in the direction of the gradual avoiding the rules of harmony and contrapunctus (Fig. 7.2). The maximum in complexity has appeared when Arnold Schönberg has completely destroyed all the rules of harmonization. Today, there are still excellent composers, but they are using the harmonic and "contrapunctic" solutions which already have been well established in the history of music. Can the Art still continue?

Both the principles of the "limitology", the maximum of the combinatorial complexity that appears between the simplicity and chaos, as well as the maximum in

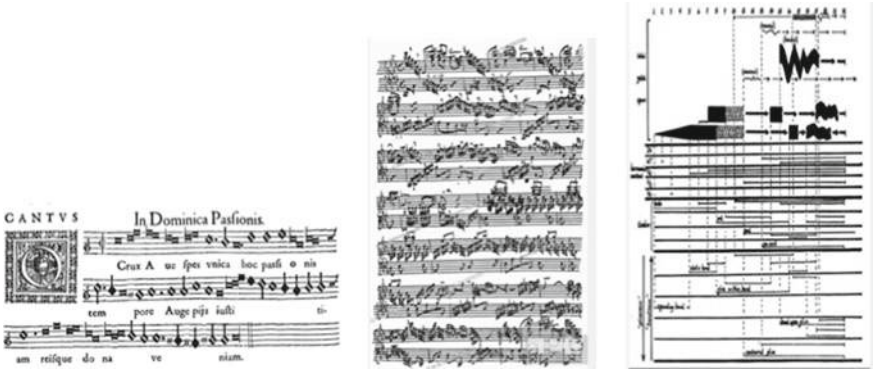

Fig. 7.2 Limits of complexity in music. (From left to right: G. P. da Palestrina, J. S. Bach, and K. Penderecki)

Fig. 7.3 Limits of complexity in the fine art. (From left to right: Picasso's *Bull's Head*, and its transformation to the reductionistic sum of some bicycle parts)

the synchronic complexity which follows from the principle of the diminishing interactions (Sect. 4.1) could be used among the possible criteria for the distinguishing of the work of art from other creations. The work of art could be represented as a peak of maximum complexity, similarly as it is in all of the correlations of complexity with the diversity (entropy) represented in this book. The minimal change in the structure of the work of art in any directions, either to the simplicity to the continuous chaos, respectively, would destroy its inherent complexity. Imagine, what could appear if the Picasso's *Bull's Head* is replaced with the completely reductionistic "sculpture" represented on the right side of the Fig. 7.3?

References

1. McGhee GR (2019) Convergent evolution on Earth. MIT Press, Cambridge, London
2. Pearce T (2012) Convergence and parallelism in evolution: a neo-Gouldian account. Brit J Philos Sci 63:429–448
3. Crutchfield JP (2003) What lies between order and chaos. In: Casti J, Karlqvist A (eds) Art and complexity. Elsevier Science B.V.
4. Edmonts B (1999) Syntactic measures of complexity. Doctoral thesis, University of Manchester, U.K.
5. Barrow JD, Tipler F (1986) The anthropic cosmological principle. Oxford University Press

Chapter 8
Concluding Remarks

In this work, the relationship between the phenomena of complexity and the theory of systems is clarified starting with the discussion about the nature of the term "complexity". The complexity of an entity (also called the "actuality") appears as a combination of three components: synchronic, diachronic, and combinatorial complexity. The possibility of the limits of complexity is explained for all of the three components. As synchronic or structural complexity depends on the energy of interactions during the formation of particles of higher complexity level from the components on the lower level, the most complex structures consist from the entities that are bound to each other so loosely that the formation of the higher complexity level is not probable. This intention of the synchronic complexity to disappear is formulated as the *principle of diminishing interactions*. Limits of diachronic and structural complexity stems from the analysis of the relationship between diversity (represented by Shannon entropy) and complexity. From the theory of cellular automata how it is represented by S. Wolfram, the maximal complexity of patterns appears not when the diversity (entropy) reaches its maximum, but rather for the patterns whose variation in the structure causes the highest change in entropy. The same conclusion follows also from other examples represented in this book. In summary, the maximum of complexity appears in the state in which the Shannon entropy, as well as the fractal dimension reach the value of the Golden ratio. Interestingly, Shannon entropy, the critical fractal dimension and the first Feigenbaum constant are in the simple mathematical relationships. This fact has led us to the new definition of the limits of diachronic and combinatorial complexities as the *state of organization of the actuality, whose minimal variation causes maximal change in entropy*. Thus, when entropy is defined as a measure of order/disorder, complexity is defined as a state of organization. This statement is in the contrast with the concepts about complexity which are derived either from the investigations of evolution (for instance, Ref. [1]), or from Simon's investigation of economic and social systems [2]. In the wide literature prevails the opinion that complexity and diversity are identical categories. By argumentation represented in all the chapters of this work, I argue that complexity

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is not the diversity, rather it is an authentic category. In addition, the most complex structures are not the states on the thermodynamic equilibrium. It seems that the highest complexity belongs to the structures which represent the transition states which appear during the transformation of the starting arrangements to the product structures.

Systems are defined as consisting of the entities (actualities) which have their position within the three component "complexity space" (synchronic, diachronic, and combinatorial). In the system, the actualities are variously interconnected. As such, the system can be represented as a topological object by using graph theory. The graphs representing systems are mathematically interpreted as "adjacency matrices" and their determinants. The development of the determinant led to the polynomial which has the solutions that are known as a spectrum of the graph. It is argued how such graph theoretical interpretation of systems could provide a new view on the teleological problem of function to which the system should be adapted. The appearance of all the systems is caused by the pressure of the environment. Such pressure is manifested as function. Systems are formed to perform this function, independently whether this function is in the nature, or, if this function is a sort of technical design. Accordingly, systems are teleologically determined. Finally, what is the relationship between the theory of complexity and the theory of systems? Simply, when systems are dynamical space-temporal objects, complexity defines their particular *state of organization.* However, epistemologically, both the theories overlap.

References

1. Brooks DR, Willey EO (1988) Evolution as entropy. The University of Chicago Press, Chicago, London
2. Simon HA (1999) The sciences of the artificial. The MIT Press, Cambridge, Massachusetts, p 128

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